Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

April 10, 2017

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New Tool for Interactive Exploration of Multi-Petabyte Global Ocean Time-Series Data

- Until now, scientists from JPL and MIT have been unable to examine their extremely large dataset in its entirety, due to sheer size and complexity: 4-plus petabytes of 1/48° time-varying, multivariate data on a 22-billion point domain, representing our best global state estimate of ocean dynamics.
- A new Ames hyperwall tool developed by the HECC Visualization team allows scientists to interactively explore their entire dataset on time scales of their choosing, and to follow up immediately on hunches, with detailed custom-tuned multivariate views of any part of the time series—*an unprecedented capability for data of this size*.
- Scientists are now able to combine views of multiple, time-varying diagnostic and prognostic variables in various ways in order to interrogate dynamic relationships at the limit of the data resolution.
- The JPL/MIT team particularly liked the ability to plot evolving quantities as evolving scatter plots, with brushable selections linked to other scatter plots and to standard latitude-longitude views. JPL's Jinbo Wang commented: "The new tool of exploring ocean physics in parameter space (scatter plot) unlocks the door to a new world of ocean data exploration."
- All of these capabilities leverage the unrivalled network bandwidth and data access/processing capabilities of the Ames hyperwall, and represent the state-of-the-art in interactive visualization and data analysis.

Mission Impact: In one day of using the new tool on the hyperwall, ECCO scientists from NASA's Jet Propulsion Laboratory found four features in the ocean data that could lead to publishable results.

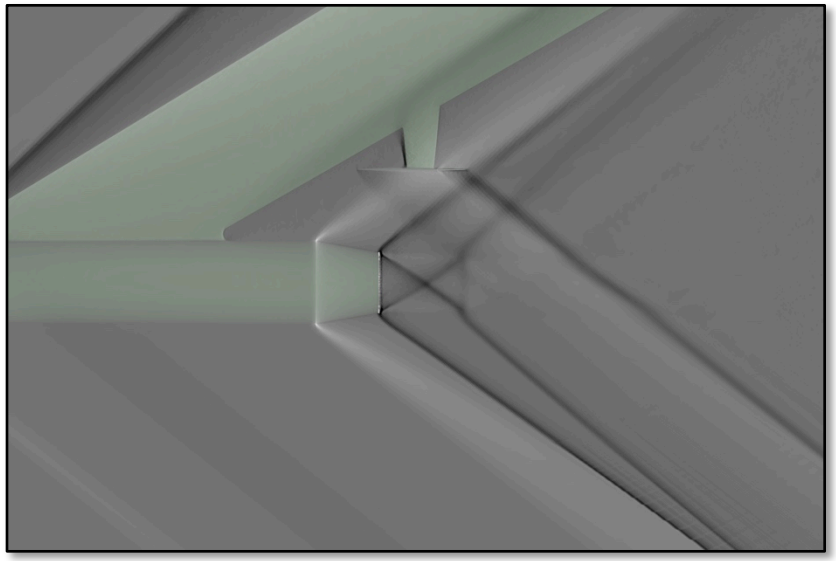
Ocean scientists from NASA's Jet Propulsion Laboratory use the updated HECC visualization tool on the hyperwall to correlate salt concentration with temperature across a dataset from a global ocean simulation at a resolution of 1/48°.

POCs: David Ellsworth, david.ellsworth@nasa.gov, (650) 604-0721, NASA Advanced Supercomputing (NAS) Division, CSRA LLC; Chris Henze, chris.henze@nasa.gov, (650) 604-3959, NAS Division

Visualization Team Develops New Computational Schlieren Capability

- The HECC Visualization team recently developed a new computational Schlieren visualization technique for polyhedral data produced by the Launch Ascent and Vehicle Aerodynamics (LAVA) flow solver. Their results match well with experimental Schlieren images from similar configurations.
- The LAVA results correspond to experimental studies conducted by the NASA Ames Wind Tunnel Systems Branch.
- Supporting LAVA unstructured polyhedral output required several extensions to the visualization infrastructure:
  - Added support for polygon and polyhedron cells and meshes based on those cell types.
  - Adopted Intel's Open Source Embree library for accelerated ray-casting calculations in unstructured data.
- The team anticipates being able to further extend this capability to support other grid types, such as overset curvilinear grids.

Mission Impact: HECC's new visualization capability enables more effective comparisons between Schlieren images produced by wind tunnel experimentalists and corresponding configurations modeled by computational scientists.



The new computational Schlieren technique was used to visualize shocks induced by supersonic flow from a nozzle, based on a LAVA polyhedral mesh solution. The configuration models the tail end of a supersonic aircraft. Note the horizontal surface above the nozzle, which corresponds to one horizontal stabilizer design candidate, and the reflected shock.

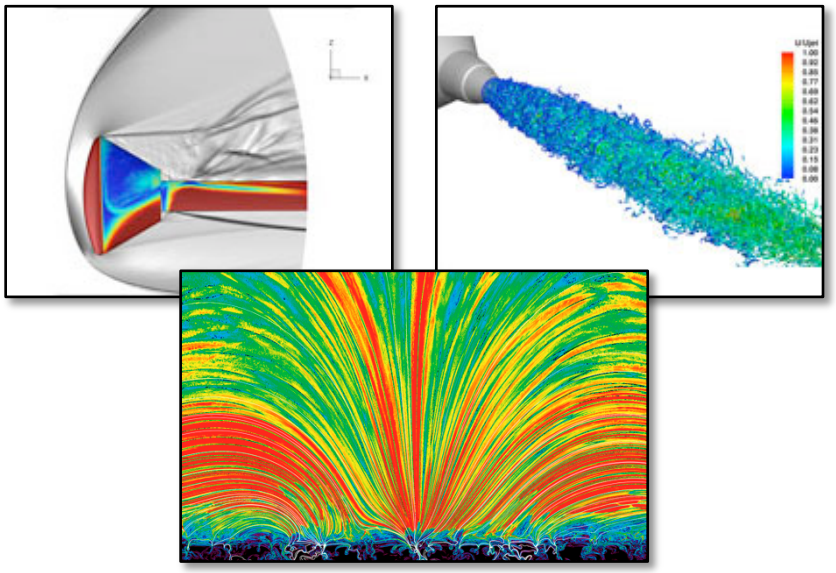
POCs: Patrick Moran, patrick.moran@nasa.gov, (650) 604-1660, and Marie Denison, marie.f.denison@nasa.gov, (650) 604-5588, NASA Advanced Supercomputing (NAS) Division

HECC Supercomputer Usage in March 2017 Sets New Record of Over 24 Million SBUs

- In March, the combined usage on HECC supercomputers set a new record of 24,483,414 Standard Billing Units (SBUs*).
- Usage of Pleiades, Electra, Merope, and Endeavour by 340 science and engineering projects from across NASA contributed to this record.
- Usage exceeded by over 1.7 million SBUs the previous record of 22,757,811 SBUs set in January 2017.
- This increase was enabled by high demand, system stability, and efficient operations that delivered system utilization of over 85% (where 75% utilization is the target).
- The top 10 projects used from 520,417 to 2,881,797 SBUs each, and together accounted for over 37% of the total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node.*

Mission Impact: Increasing capacity of HECC systems provides mission directorates with more resources for the accomplishment of their goals and objectives.



Images representing computing projects from different mission directorates. Clockwise from top left: (1) Simulation of a wind tunnel model of the Orion capsule. *J. Brock, NASA/Ames* (2) Turbulent shear layer caused by the mixing of a high-speed jet with slow-moving ambient air. *J. Housman, NASA/Ames* (3) Simulation of heating patterns in the solar atmosphere. *J. Martinez-Sykora, Lockheed Martin Solar & Astrophysics*

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

APP Team Updates Applications Used to Measure Computer Resource Usage

- The HECC Application Performance and Productivity (APP) team recently finished an extensive update of five of the six benchmark applications used to establish the System Billing Unit (SBU) on HECC compute resources.
- The last update of the benchmarks, based on Intel Westmere processors, occurred in 2011. Updating the suite makes it more representative of current production workloads and state-of-art hardware.
- The NAS portion of the HECC SBU suite consists of applications from space sciences (Enzo), computational fluid dynamics (FUN3D, OVERFLOW, USM3D), and climate/weather modeling (nuWRF).
- For each of the five applications, APP obtained the most recent version of code and chose a dataset reflecting the size of typical runs. The team then tuned the specific run for the SBU measurement to be representative of production use of HECC resources.
- A sixth code, GEOS-5, is being updated at NCCS. Once that is done, APP will measure its performance and establish new base rates for compute resources provided by HECC and NCCS.

Mission Impact: By establishing charging rates that reflect the power of resources to compute the NASA workload, HECC ensures that user demand across the various resource types will be balanced.

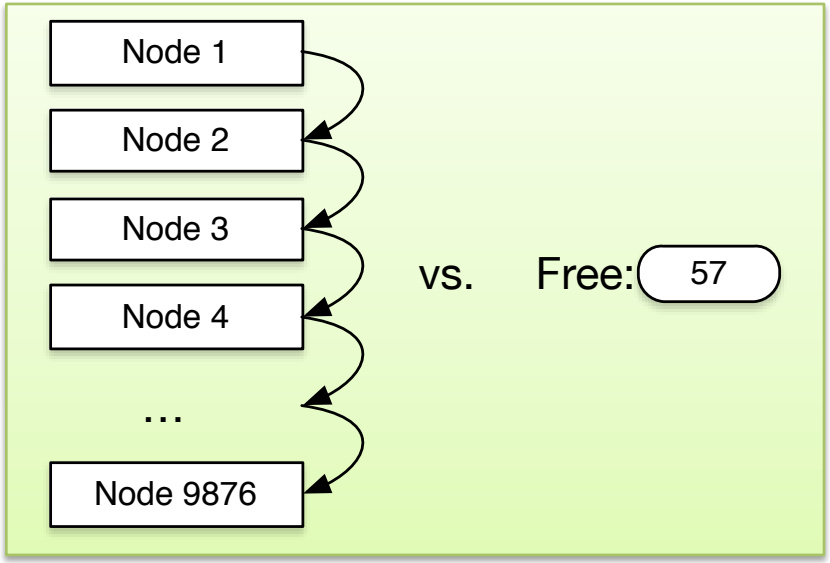
HECC's Application Performance and Productivity team measures the effectiveness of different node types at computing a typical NASA workload in order to establish fair charging rates for use of the resources.

POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing (NAS) Division;
Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NAS Division, CSRA LLC

Job Scheduler Prototype Validates Algorithm Designed by HECC Staff

- Altair released a prototype PBSPro scheduler implementing a job scheduling algorithm designed by an HECC Supercomputing Systems staff member.
- The prototype scheduler performed up to 15 times faster than the current production scheduler, validating the algorithm designed for large clusters such as Pleiades and Electra.
- Increased scheduler performance allows better utilization of Pleiades and Electra, enables use of additional scheduling features that provide flexibility to users, and should also make it possible to drop from the current dual-scheduler setup to a single scheduler.
- Altair was tasked with generating a fully functional scheduler that incorporates the algorithm for production use on Pleiades and Electra.

Mission Impact: The prototype implementation of a new algorithm for scheduling the work done on Pleiades and Electra demonstrated significant performance improvement, setting the stage for improved utilization of the HECC computational capability.



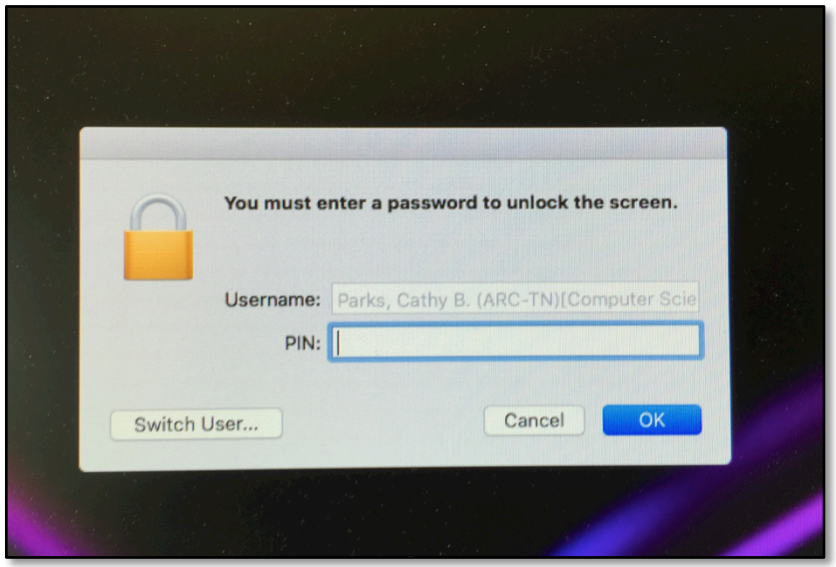
A computationally inexpensive approach that eliminates most searches through lists of nodes has demonstrated a significant improvement in scheduling speed.

POCs: Dale Talcott, dale.r.talcott@nasa.gov, (650) 604-0555, and Greg Matthews, gregory.a.matthews@nasa.gov (650) 604-1321, NASA Advanced Supercomputing Division, CSRA LLC

ESS Team Provides Centrify Consulting to Agency Mac Support Organizations

- After a successful roll out of Centrify for PIV authentication on NAS Macs, the HECC Engineering Servers and Services (ESS) team was called on to assist other agency support groups with their Macs.
- For the Centrify rollout, ESS developed tools and worked through issues to stabilize PIV authentication, including:
  - Completed an Organizational Unit (OU) setup for Centrify.
  - Developed FileVault boot account and FileVault password management code.
  - Defined an automated process to switch between NDC and PIV credentials for badge issues.
  - Overcame wireless lockout conditions.
- ESS met with Agency Consolidated End-user Services (ACES) and non-ACES engineers from HQ, Goddard, and Ames to explain the processes, provide documentation and code, and answer questions about the Centrify solution.

Mission Impact: Supporting other engineering teams with their Centrify rollout efforts will help to make agency Macs more secure through the use of PIV authentication.



PIV authentication on the Mac is managed by the Centrify application and requires entry of the user's PIN associated with their NASA badge.

POC: Cathy Parks, cathy.b.parks@nasa.gov, (650) 604-4314, NASA Supercomputing Division, CSRA LLC

Annual Independent Security Assessment Leads to Renewal of HECC Authorization to Operate

- On March 10, 2017 the Ames Research Center Deputy Center Director, as the Authorizing Official for the NAS security plan, signed the fully-acceptable Authorization to Operate (ATO) for all NAS (including HECC) systems.
- The approved ATO is the final step in the annual security assessment required of all NASA systems.
- The annual assessment must be conducted by an independent assessor.
- The assessor evaluates the compliance of the facilities, systems, and operations under the NAS Supercomputing Storage and Support Systems (NS4), CD-9999-M-ARC-3232 security plan that covers the NAS Division systems, including HECC systems.
- The ATO ensures the continued operation of HECC systems in compliance with NASA security requirements.

Mission Impact: The Authorization to Operate allows HECC supercomputers and support systems to continue to operate, and the independent assessment provides an important confirmation of the security compliance of HECC systems.

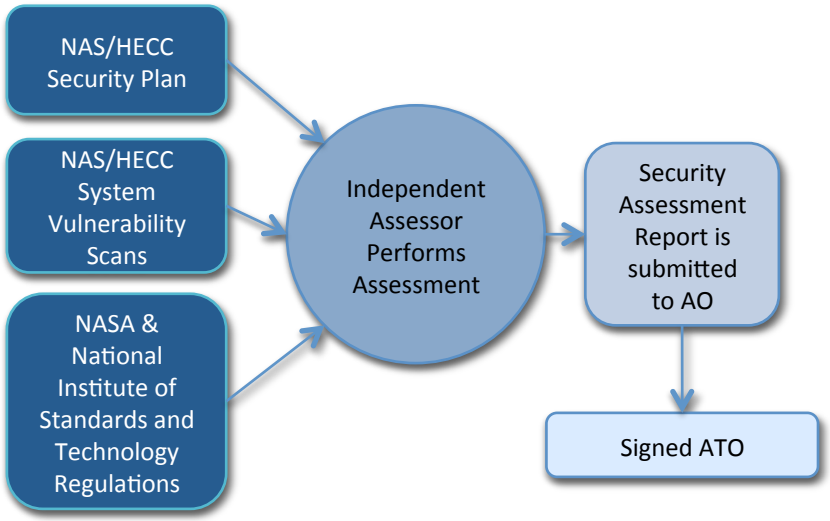


Chart showing the flow of information used by the independent security assessor to produce an annual security assessment report, which is submitted to the authorizing official to award a renewal of the authorization to operate.

POC: Thomas Hinke, thomas.h.hinke@nasa.gov, (650) 279-4053, NASA Advanced Supercomputing Division

HECC Property Management Achievements in 2016

- Property custodians responsible for HECC/NAS property tracked over 1,350 pieces of decaled equipment with a value of over $123.6 million. Each piece of equipment requires numerous updates through the life cycle of its use.
- Equipment management activities for 2016 included:
  - Successful completion of the 2016 annual inventory.
  - Disposal of 177 pieces of tagged equipment with a value of over $1.6 million.
  - Decaling of about 200 items and adding RFID tags to current equipment.
  - Resolution of over 800 Remedy tickets for property management activities.
  - Completion of hundreds of property forms for equipment ownership, property passes, excess, location changes, shipping forms, and forms for international travel with government equipment.
- The Property staff's active tracking and updates of HECC/NAS equipment helps to ensure a successful annual inventory.

Mission Impact: At NASA's largest supercomputing facility, accurate tracking of assets through their life cycles and tracking of data removal during system disposal ensure good control of government equipment and prevents loss of NASA data.

HECC property custodians track the acquisition, movement, and disposal of all NAS facility decaled equipment, including the Pleiades supercomputer components.

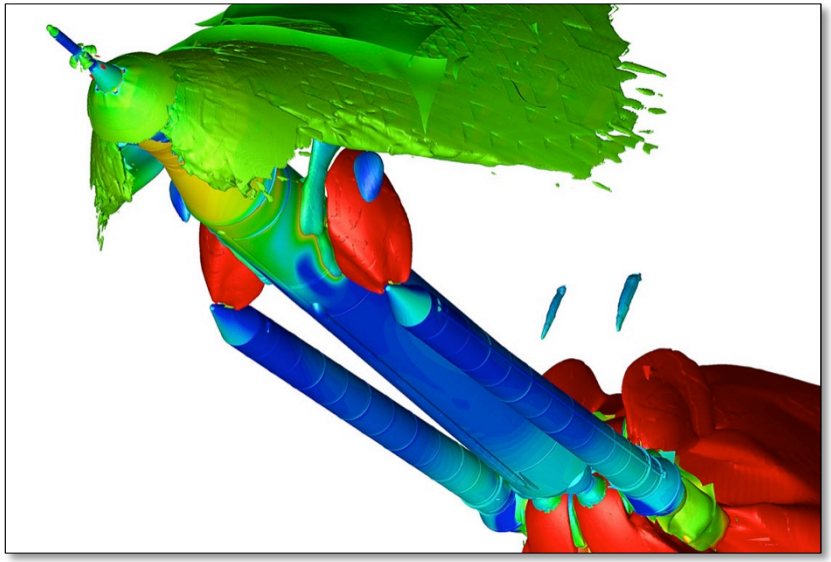
POCs: Judy Kohler, judy.j.kohler@nasa.gov, (650) 604-4303, and Chacky Tsan, chacky.s.tsan@nasa.gov, (650) 604-6401, NASA Advanced Supercomputing Division, CSRA LLC

Building CFD-Based Aerodynamic Databases for the Space Launch System *

- Researchers are running computational fluid dynamics (CFD) simulations on Pleiades and Electra to quantify the aerodynamic forces during the ascent of the Space Launch System (SLS) and provide data to build aerodynamic databases, including:
  - Surface pressures used in venting and other dynamic analysis.
  - Distributed line loads used in structural analysis.
  - Protuberance aerodynamic loads used in vehicle design.
  - Forces and moments on the vehicle during booster separation used to verify the booster-separation system.
- One moving-body dynamic simulation of a nominal booster-separation event incorporated 22 different plumes, including 16 booster-separation motor plumes, plumes from the four core-stage main engines, and two plumes from the boosters.
- The project analyzed several different SLS vehicle designs, including multiple design iterations of the Exploration Mission-1 (EM-1) and EM-2 flight vehicles, and the cargo version of the SLS rocket.
- In the next few months, the project will provide updated databases for the EM-1 Verification Analysis Cycle 1 & EM-2 Design Analysis Cycle 2.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: CFD simulations enabled by HECC resources provide critical aerodynamic data throughout Space Launch System design cycles.



Simulation of the SLS booster separation flowfield, from a dynamic moving-body calculation with 22 plumes firing. Vehicle surface is colored by pressure contours. Isosurfaces illustrate shock waves (shown in green) and plumes (shown in red). *Jeff Onufer, NASA/Ames*

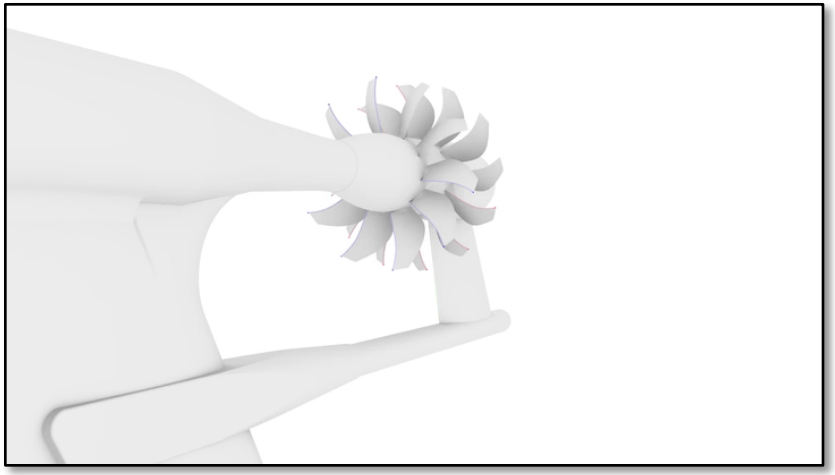
POCs: Stuart Rogers, stuart.e.rogers@nasa.gov, (650) 604-4481, NASA Advanced Supercomputing (NAS) Division; Henry Lee, henry.c.lee@nasa.gov, (650) 604-3689, NAS Division, Science and Technology Corp.

Computational Aeroacoustics for Green Aviation Propulsion Technology *

- CFD experts in the NAS Division ran first-of-a-kind aeroacoustic simulations on Pleiades to support studies of contra-rotating, open-rotor propulsion technology for its potential to reduce aircraft fuel consumption and meet airline noise standards.
- The NAS team employed higher-order accurate immersed boundary methods to simulate and analyze noise-generation mechanisms in the highly complex flow field around an open rotor. Three key tasks were performed:
  - Low-speed (landing or takeoff condition) simulations of the open rotor.
  - Open rotor installation effects simulations, which included a pylon to more closely represent how the engines are attached to airplanes.
  - Detailed analysis of the most dominant noise-generation mechanism of the open-rotor propulsion system.
- The team's higher-order methods, developed within the Launch Ascent and Vehicle Aerodynamics (LAVA) framework, demonstrated the ability to perform aeroacoustic analysis of wake-dominated flow fields; postprocessing tools allowed a detailed understanding of the noise-generation process.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: Enabled by Pleiades, these higher-order accurate simulations continue to advance the state-of-the-art in CFD simulations in green aviation for NASA's Advanced Air Transport Technology project.

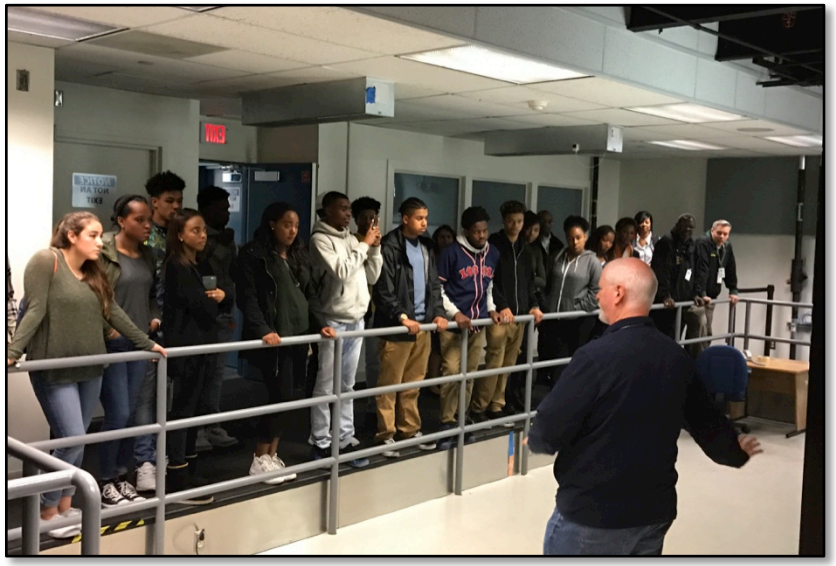


Passive particle visualization of a pylon-installed, contra-rotating, open-rotor simulation created using the Launch Ascent and Vehicle Aerodynamics (LAVA) code. Red particles are seeded on the upstream blades, and blue on the aft blades. Solid colors are seeded on the tips, while faded colors are on the blade trailing edges. *Timothy Sandstrom, Michael Barad, NASA/Ames*

POCs: Michael Barad, michael.f.barad@nasa.gov, (650) 604-0550, and Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485, NASA Advanced Supercomputing Division

HECC Facility Hosts Several Visitors and Tours in March 2017

- HECC hosted 10 tour groups in March; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - Avi Hasson, Chief Scientist of the Ministry of Economy of the State of Israel.
  - Jaya Bajpayee, Deputy Director, Science Directorate at NASA Ames.
  - A group from the Chief Information Office at HQ that visited Ames for a review of ARMD projects.
  - Francis Queen Nieto, Vice President, Raizen Energy Company; and Juan Carlos Rubio, CEO, Space Time Ventures.
  - Several members of the ECCO team from JPL and MIT held a working meeting at NAS.
  - Spring 2017 interns at Ames.
  - A group of students from Tracy High School Student Union, Tracy, CA.
  - Actress Karan Kendrick, who starred in the Hidden Figures movie, as part of her Ames tour.



Chris Buchanan (contractor lead in the NAS Division for networks, IT security, and facilities) gives an overview of the D-Wave quantum computer and the HECC capabilities to students from Tracy High School Student Union.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**Evaluation of Mixture-Fraction-Based Turbulent-Reaction-Rate Model Assumptions for High-Pressure Reactive Flows**," J. Bellan, Combustion and Flame, vol. 179, March 6, 2017.* *http://www.sciencedirect.com/science/article/pii/S0010218017300342*
- "**DeepSD: Generating High Resolution Climate Change Projections through Single Image Super-Resolution**," T. Vandal, et al., arXiv:1703.03126 [cs.CV], March 9, 2017. * *https://arxiv.org/abs/1703.03126*
- "**Thermodynamics Properties of Carbon-Phenolic Gas Mixtures**," J. Scoggins, et al., Aerospace Science and Technology, available online March 10, 2017. * *http://www.sciencedirect.com/science/article/pii/S1270963816307945*
- "**The Interaction of Finite-Width Reconnection Exhaust Jets with a Dipolar Magnetic Field Configuration**," P. Pritchett, A. Runov, Journal of Geophysical Research: Space Physics, published online March 15, 2017. * *http://onlinelibrary.wiley.com/doi/10.1002/2016JA023784/full*
- "**Fragment Acceleration Modeling for Pressurized Tank Burst**," T. Manning, S. Lawrence, Journal of Spacecraft and Rockets, vol. 54, no. 2, March 16, 2017. * *https://arc.aiaa.org/doi/full/10.2514/1.A33765*
- "**Winter Precipitation Characteristics in Western US Related to Atmospheric River Landfalls: Observations and Model Evaluations**," J. Kim, et al., Climate Dynamics, March 17, 2017. * *https://link.springer.com/article/10.1007/s00382-017-3601-5*

** HECC provided supercomputing resources and services in support of this work.*

Papers (cont.)

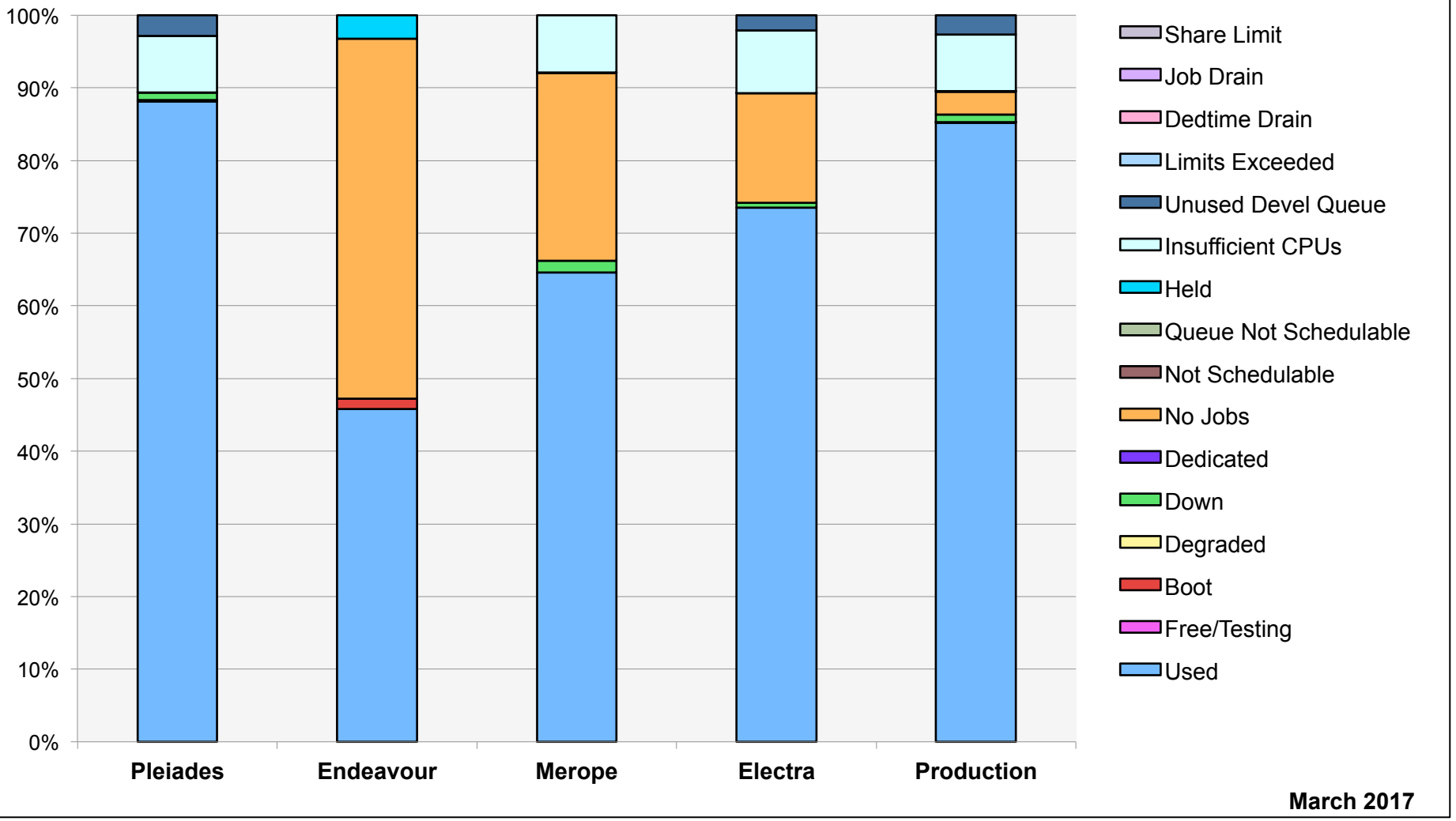
- "**The Mars Crustal Magnetic Field Control of Plasma Boundary Locations and Atmospheric Loss: MHD Prediction and Comparison with MAVEN**," X. Fang, et al., Journal of Geophysical Research: Space Physics, March 23, 2017.*
  http://onlinelibrary.wiley.com/doi/10.1002/2016JA023509/full
- "**The Impact of Clustering and Angular Resolution on Far-Infrared and Millimeter Continuum Observations**," M. Berthermin, et al., arXiv:1703.08795 [astro-ph.GA], March 26, 2017. *
  https://arxiv.org/abs/1703.08795
- "**A Search for Lost Planets in the Kepler Multi-Planet Systems and the Discovery of the Long-Period, Neptune-Sized Exoplanet Kepler-150 f**," J. Schmitt, J. Jenkins, D. Fischer, arXiv:1703.09229 [astro-ph.EP], March 27, 2017. *
  https://arxiv.org/abs/1703.09229

** HECC provided supercomputing resources and services in support of this work.*

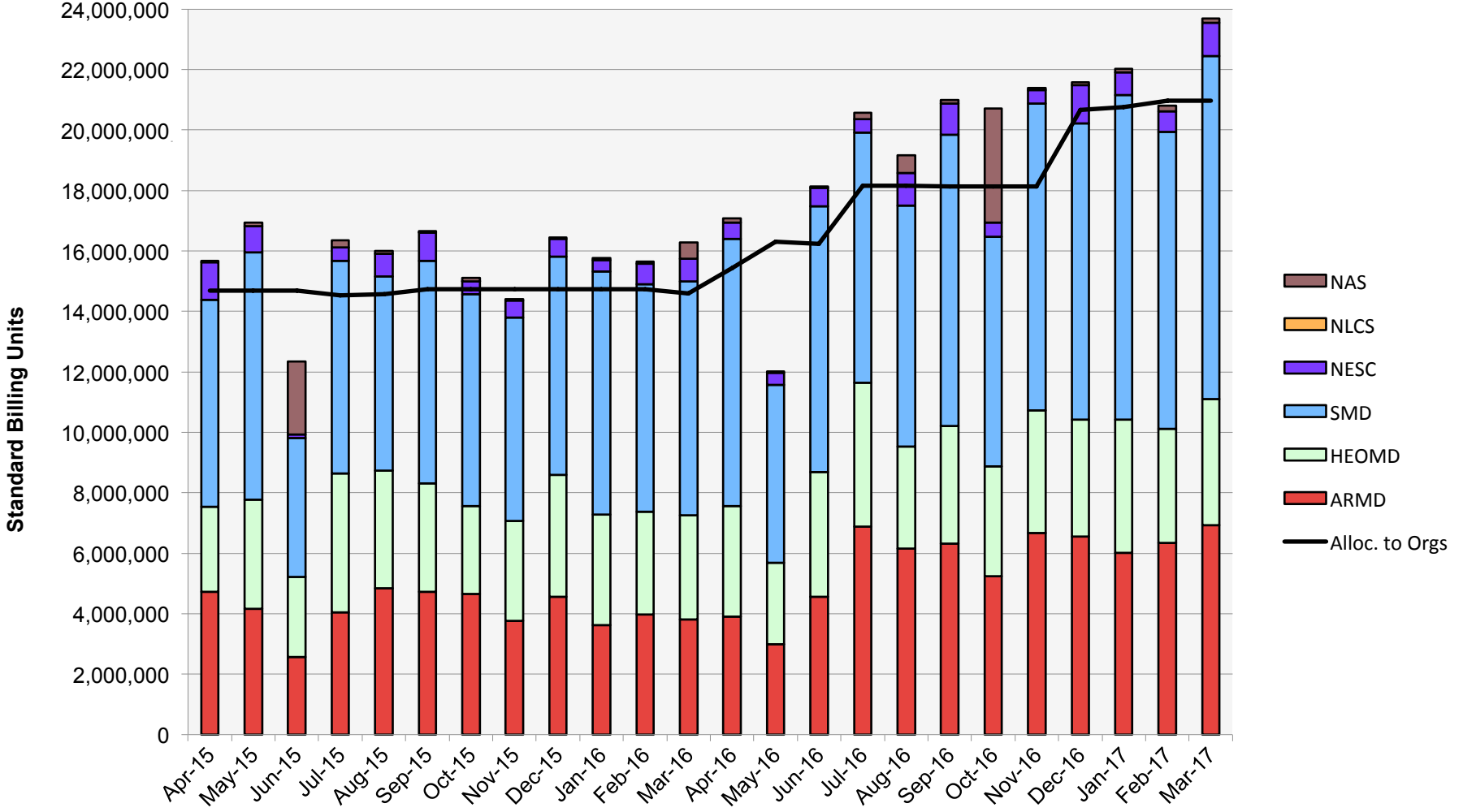
News and Events

- **Developer Spotlight: Earth Science Monitoring with Satellite Imagery**, *NVIDIA*, March 1, 2017—NASA Ames' senior research scientist, Sangram Ganguly, sits down with NVIDIA to talk about how they are using NASA's GPU-accelerated Pleiades supercomputer to analyze satellite imagery with deep learning to gain a better understanding of our planet, as part of the NASA Earth Exchange (NEX) project.
  https://news.developer.nvidia.com/developer-spotlight-earth-science-monitoring-with-satellite-imagery/
- **Quantum Computer Learns to 'See' Trees**, *Science Magazine*, March 8, 2017—Scientists are using the D-Wave 2X computer at the NASA Advanced Supercomputing facility to recognize trees, bringing researchers one step closer to using such computers for complicated machine learning problems like pattern recognition and computer vision.
  http://www.sciencemag.org/news/2017/03/quantum-computer-learns-see-trees
- **Simulating Parachute Dynamics for NASA Space Exploration Missions**, *NAS Image Feature*, March 8, 2017—Aerospace engineers at NAS are developing new, high-fidelity simulation tools to predict the complex dynamics of parachute clusters as they decelerate through the atmosphere.
  https://www.nas.nasa.gov/publications/articles/feature_parachutes_murman.html

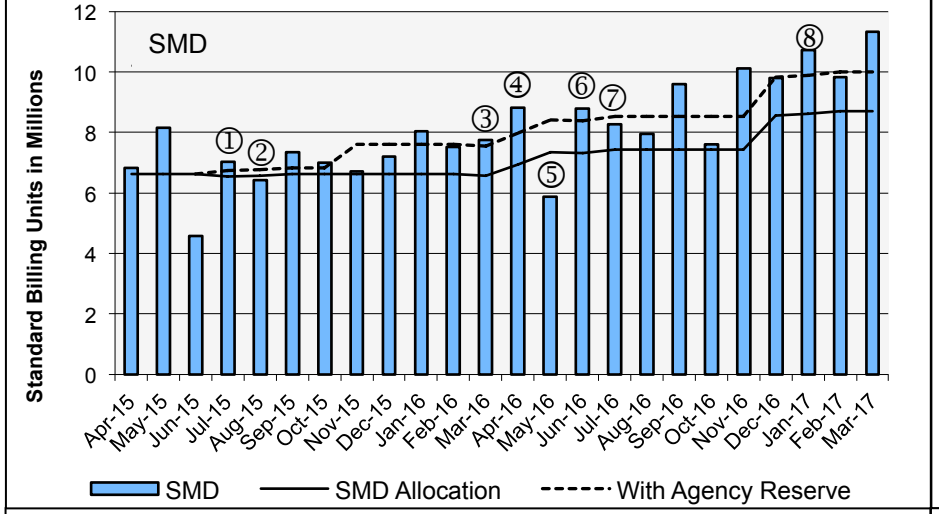
HECC Utilization

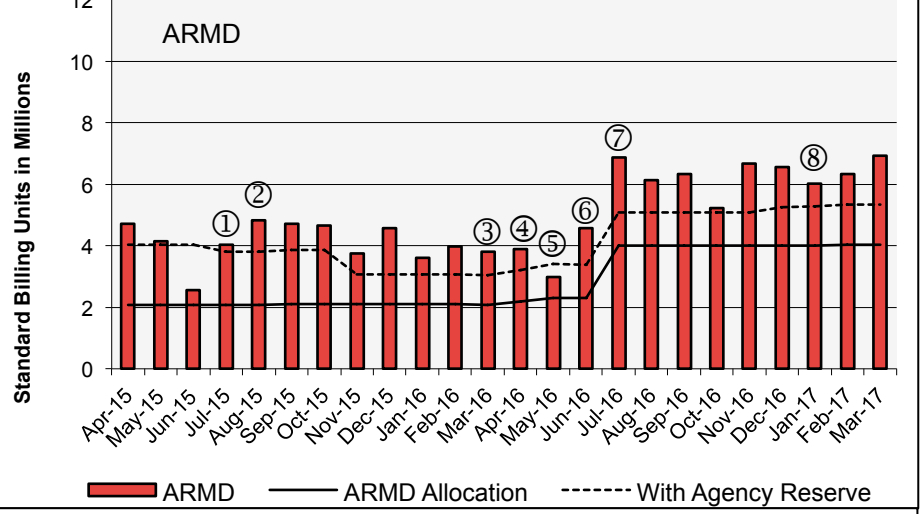


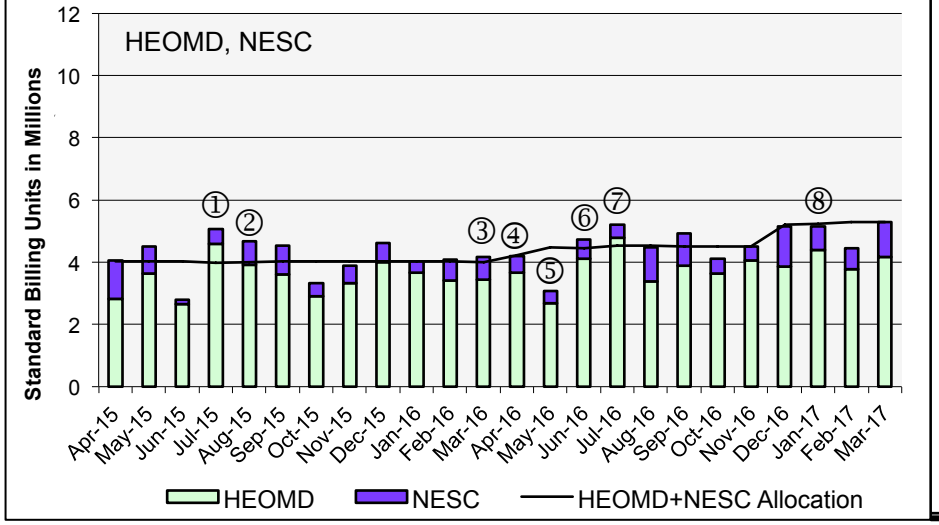
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

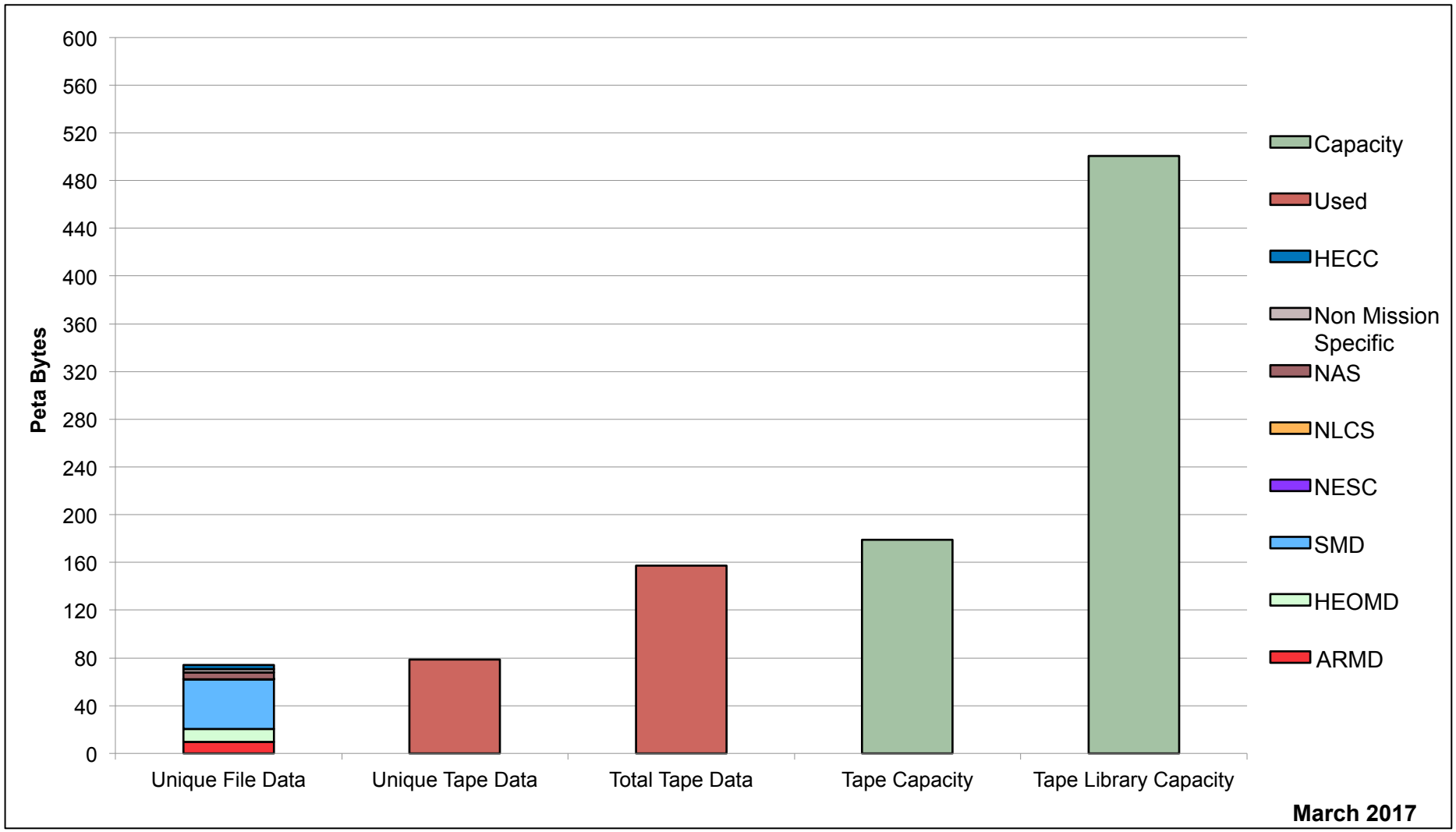






① 7 Nehalem ½ racks retired from Merope
② 7 Westmere ½ racks added to Merope
③ 16 Westmere racks retired from Pleiades
④ 10 Broadwell racks added to Pleiades
⑤ 4 Broadwell racks added to Pleiades
⑥ 14 (All) Westmere racks retired from Pleiades
⑦ 14 Broadwell Racks added to Pleiades
⑧ 16 Electra Broadwell Racks in Production, 20 Westmere 1/2 racks added to Merope

Tape Archive Status



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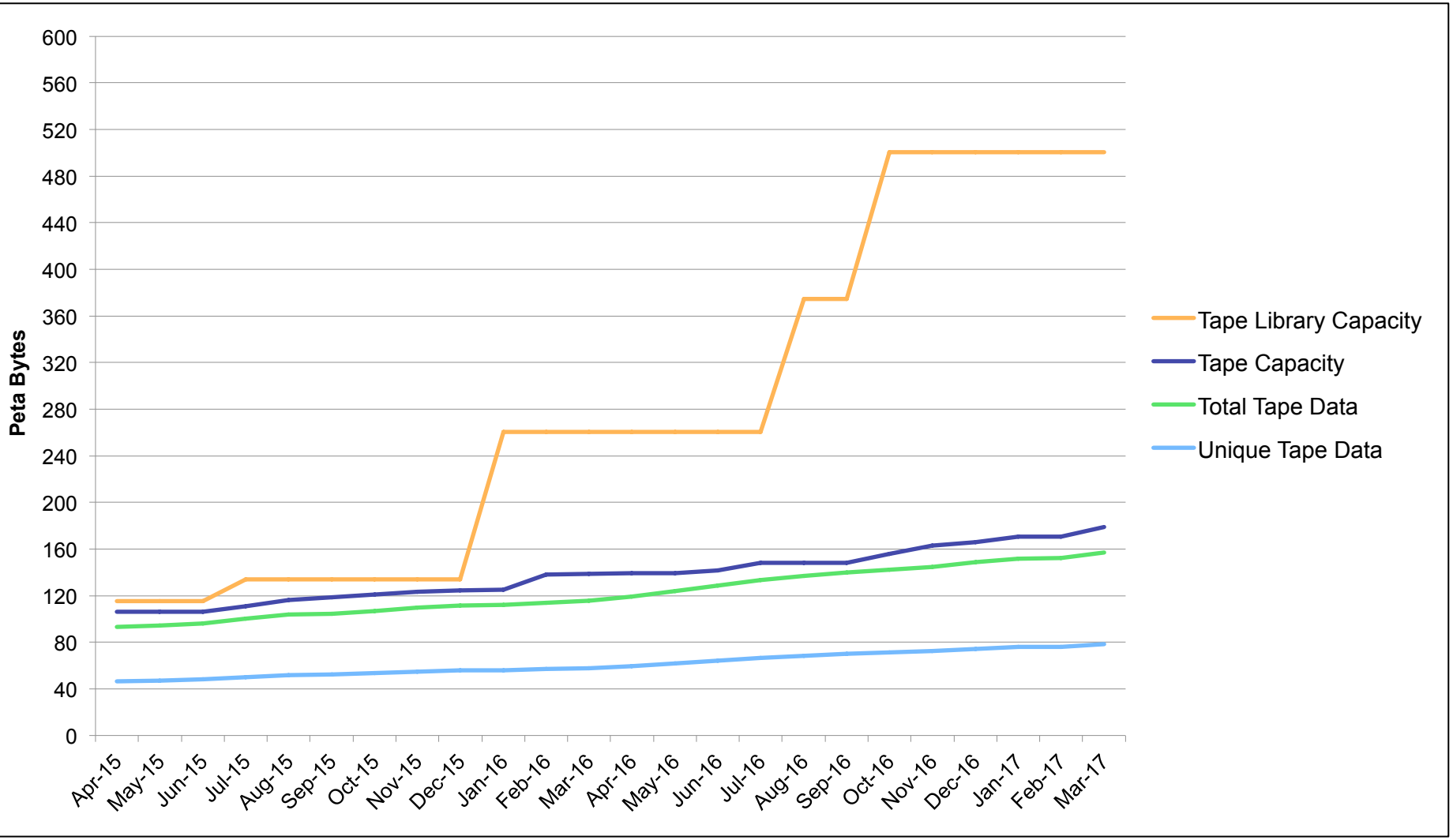
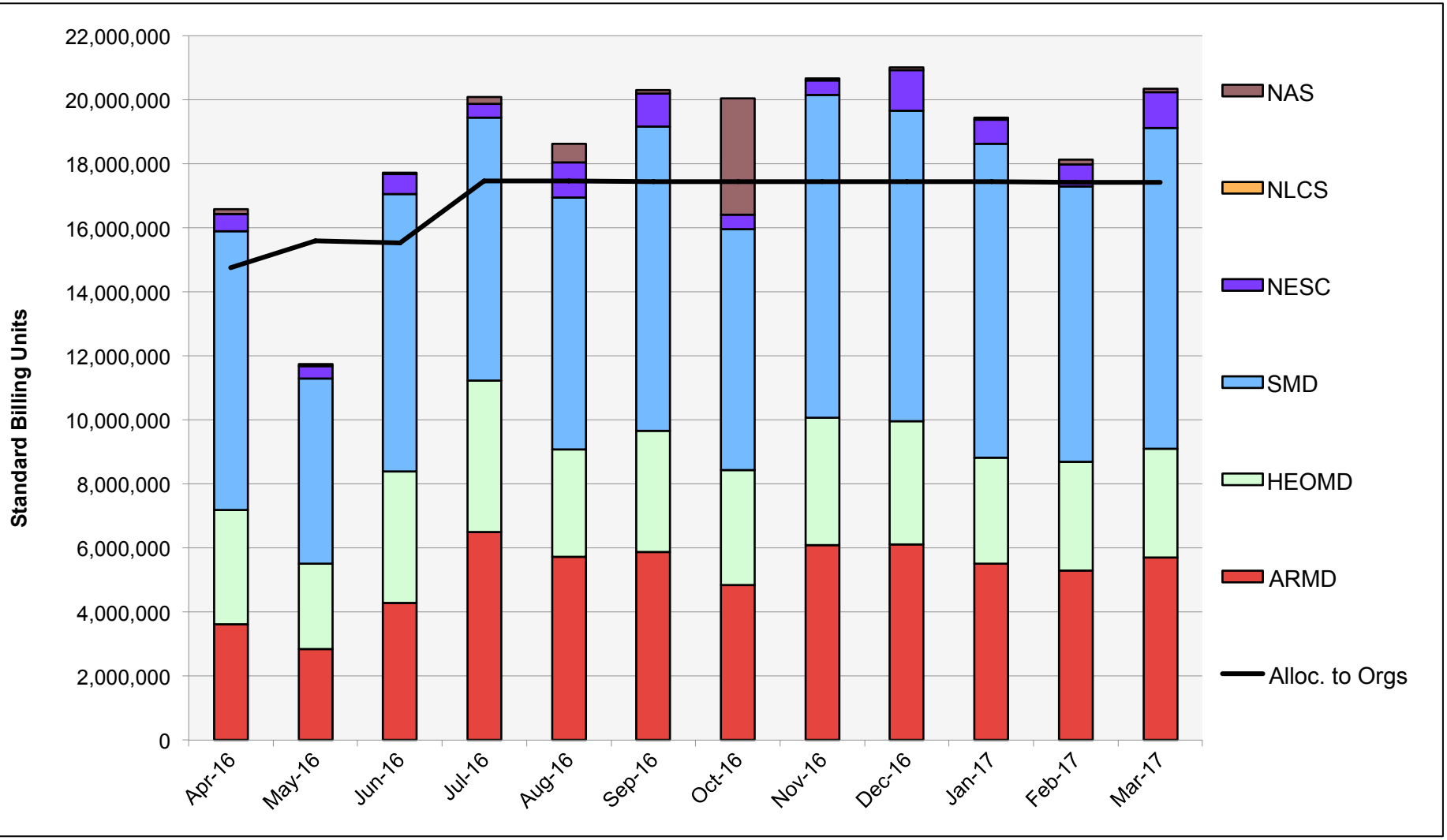
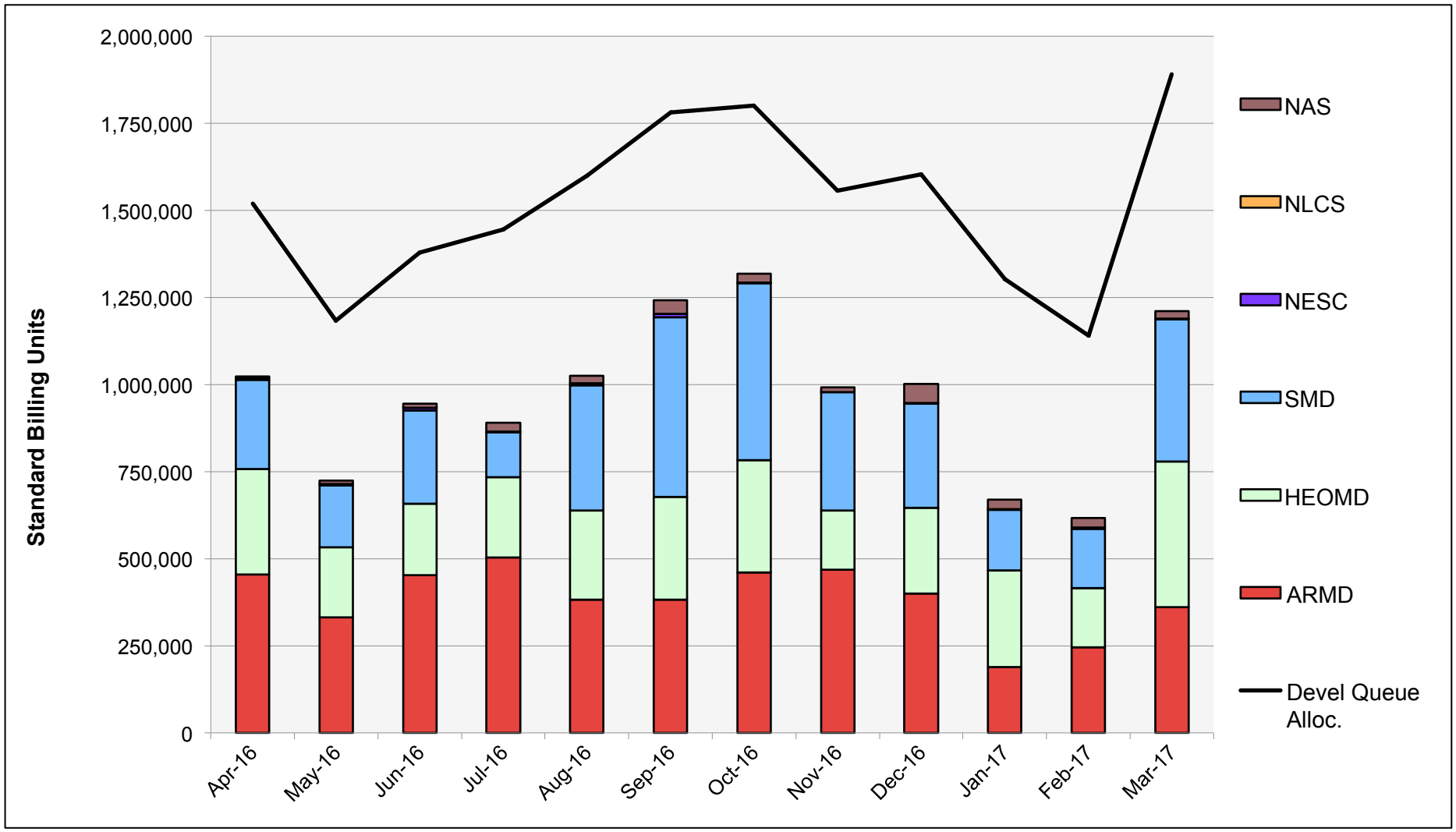


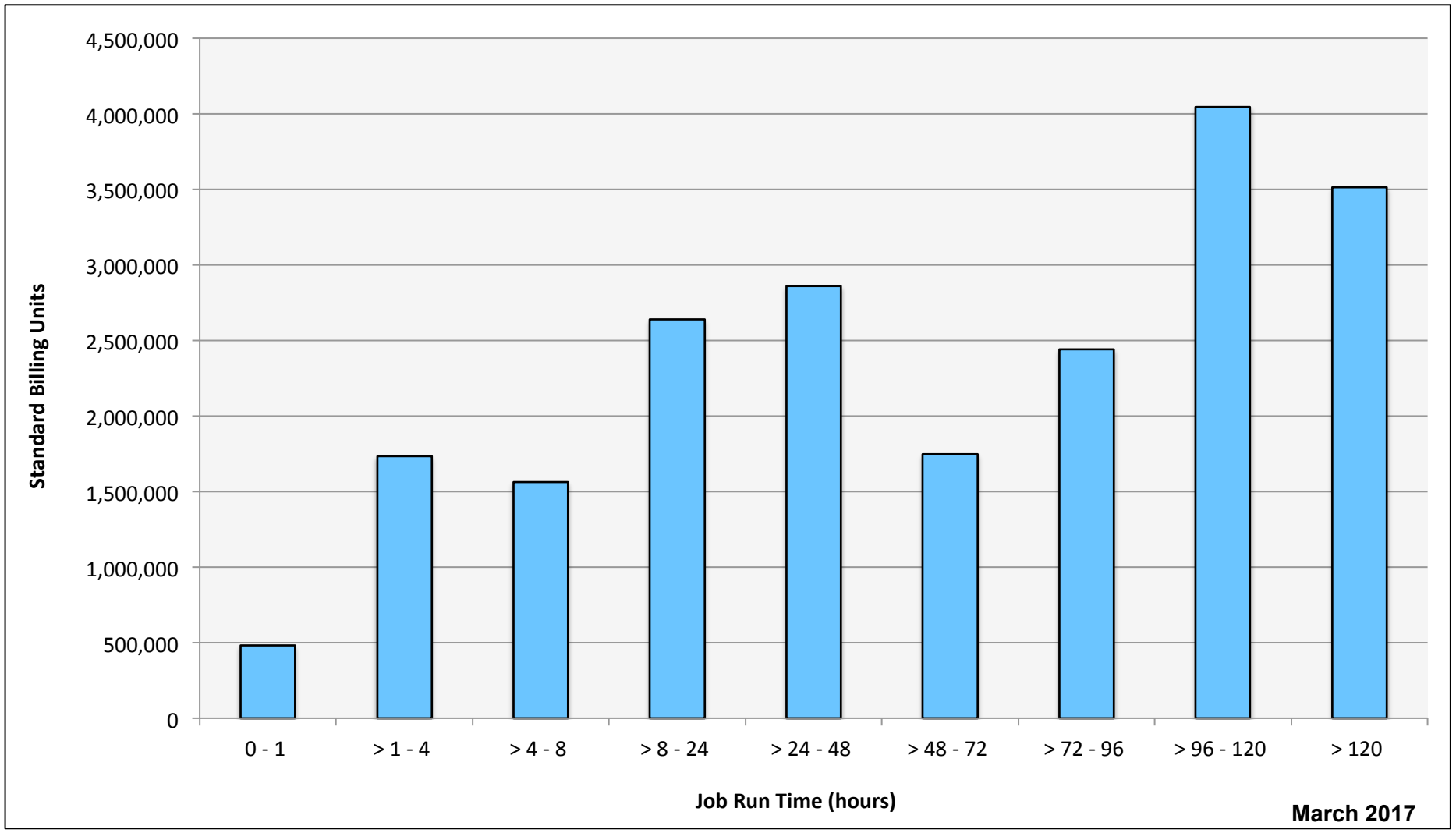
Pleiades:
SBUs Reported, Normalized to 30-Day Month



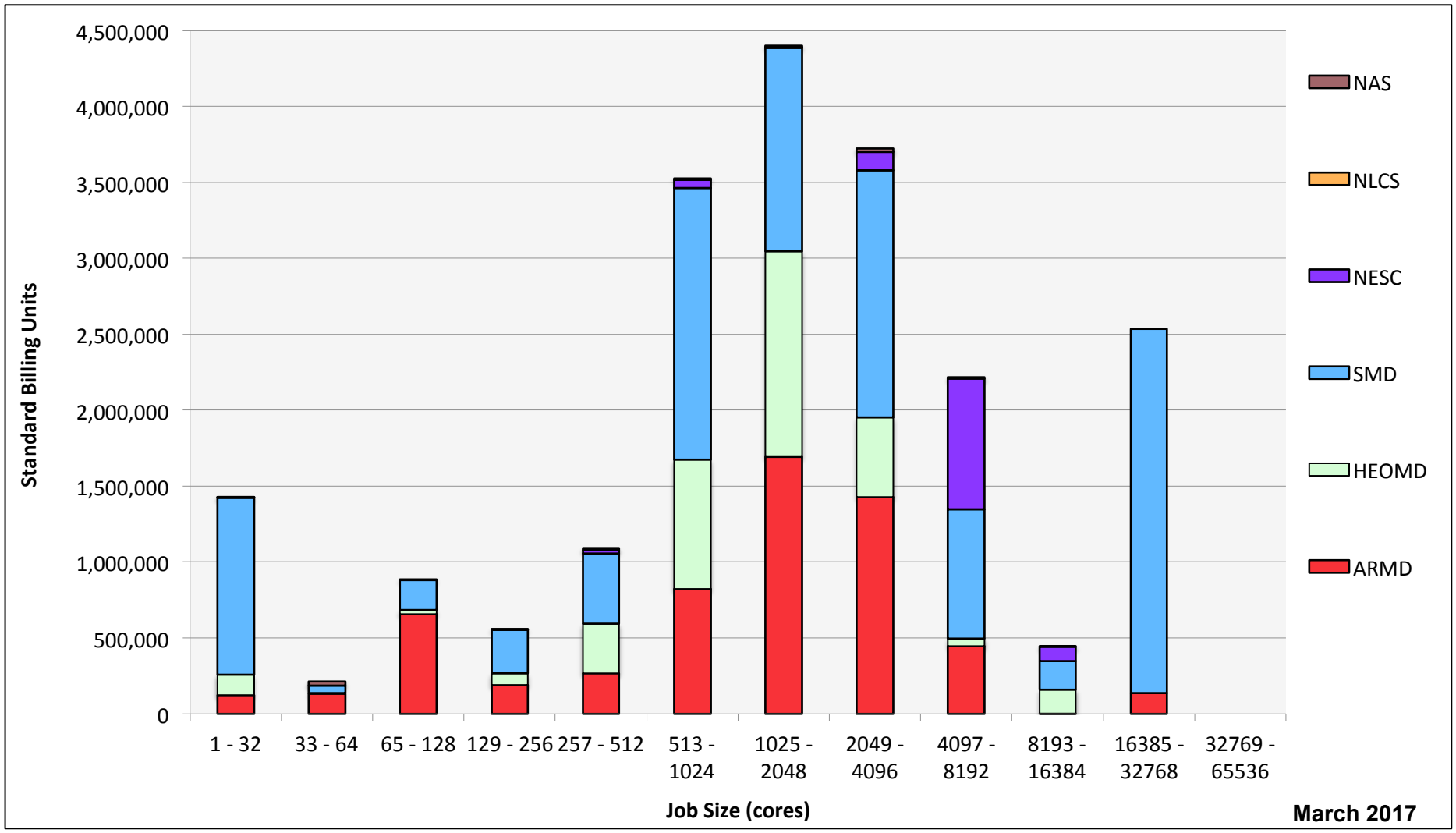
Pleiades:
Devel Queue Utilization



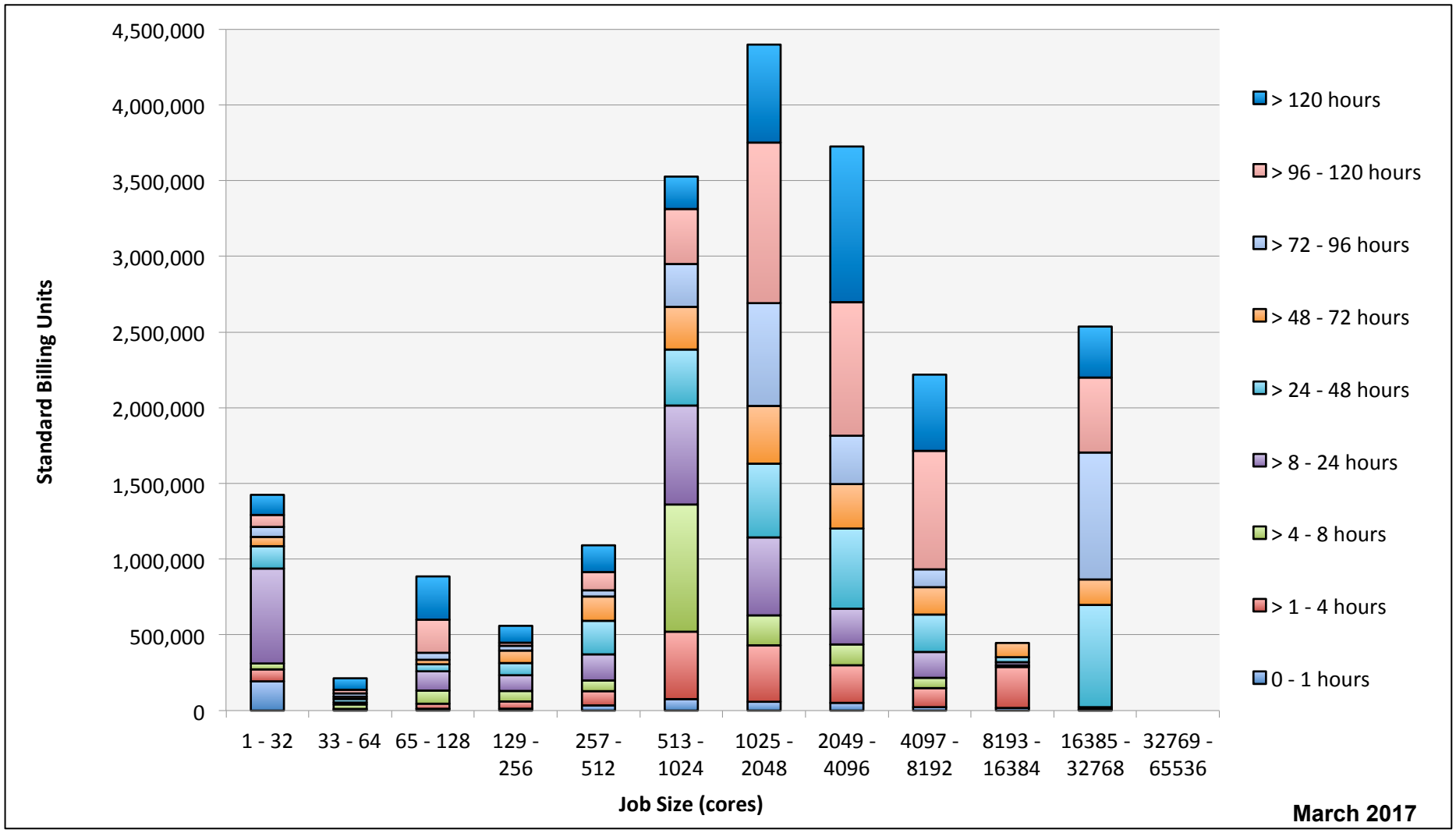
Pleiades:
Monthly Utilization by Job Length



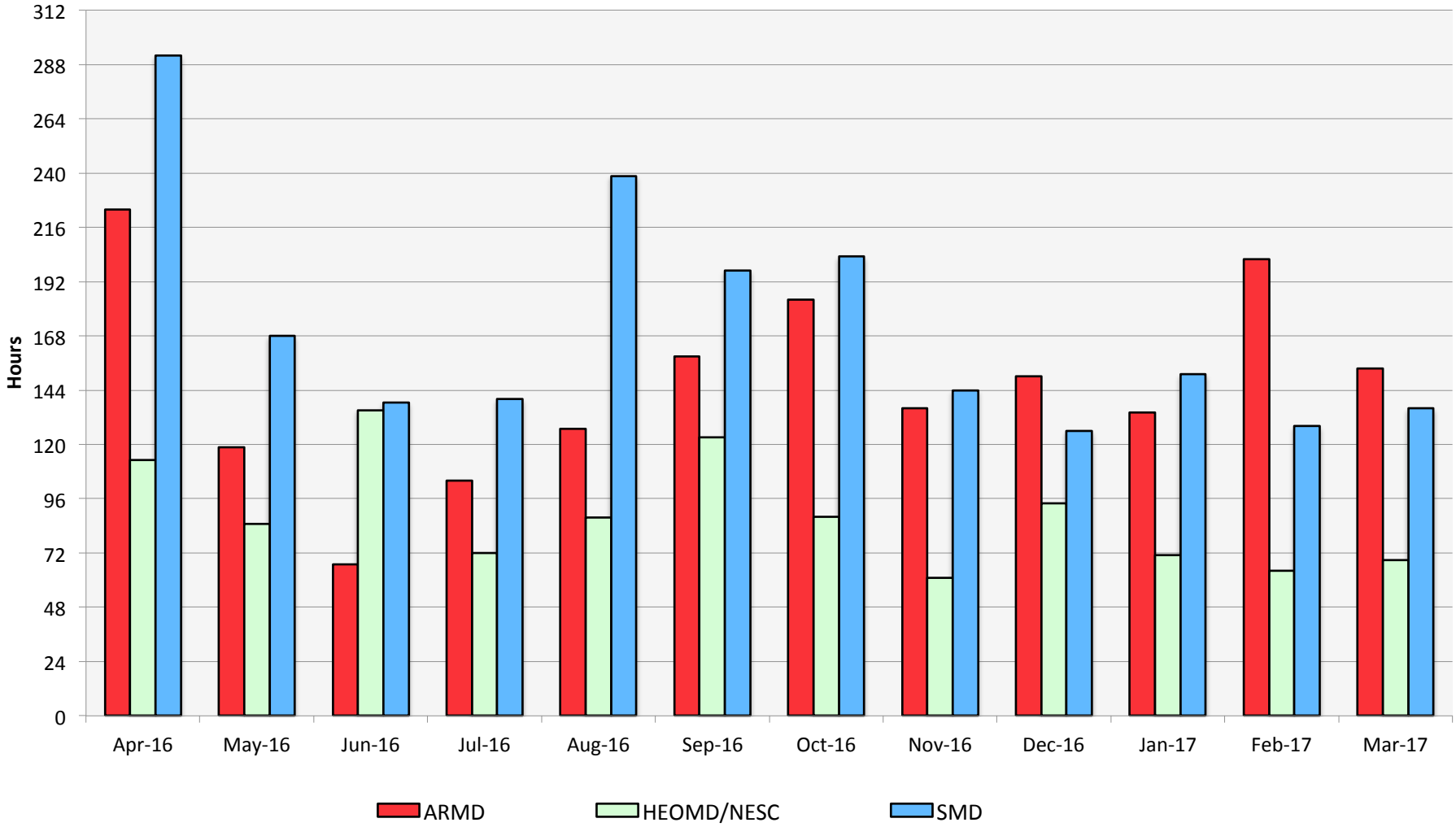
Pleiades:
Monthly Utilization by Size and Mission



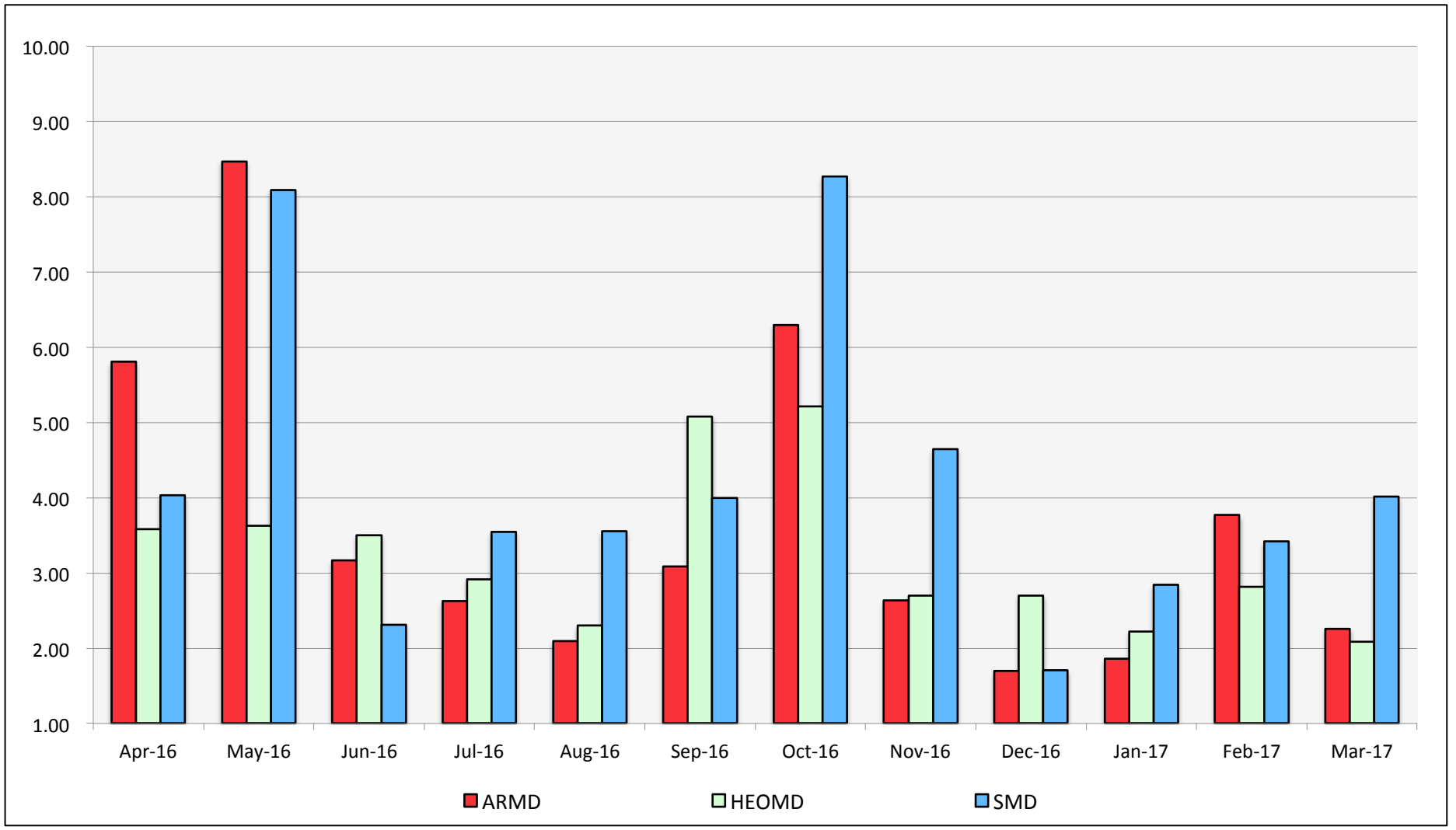
Pleiades:
Monthly Utilization by Size and Length



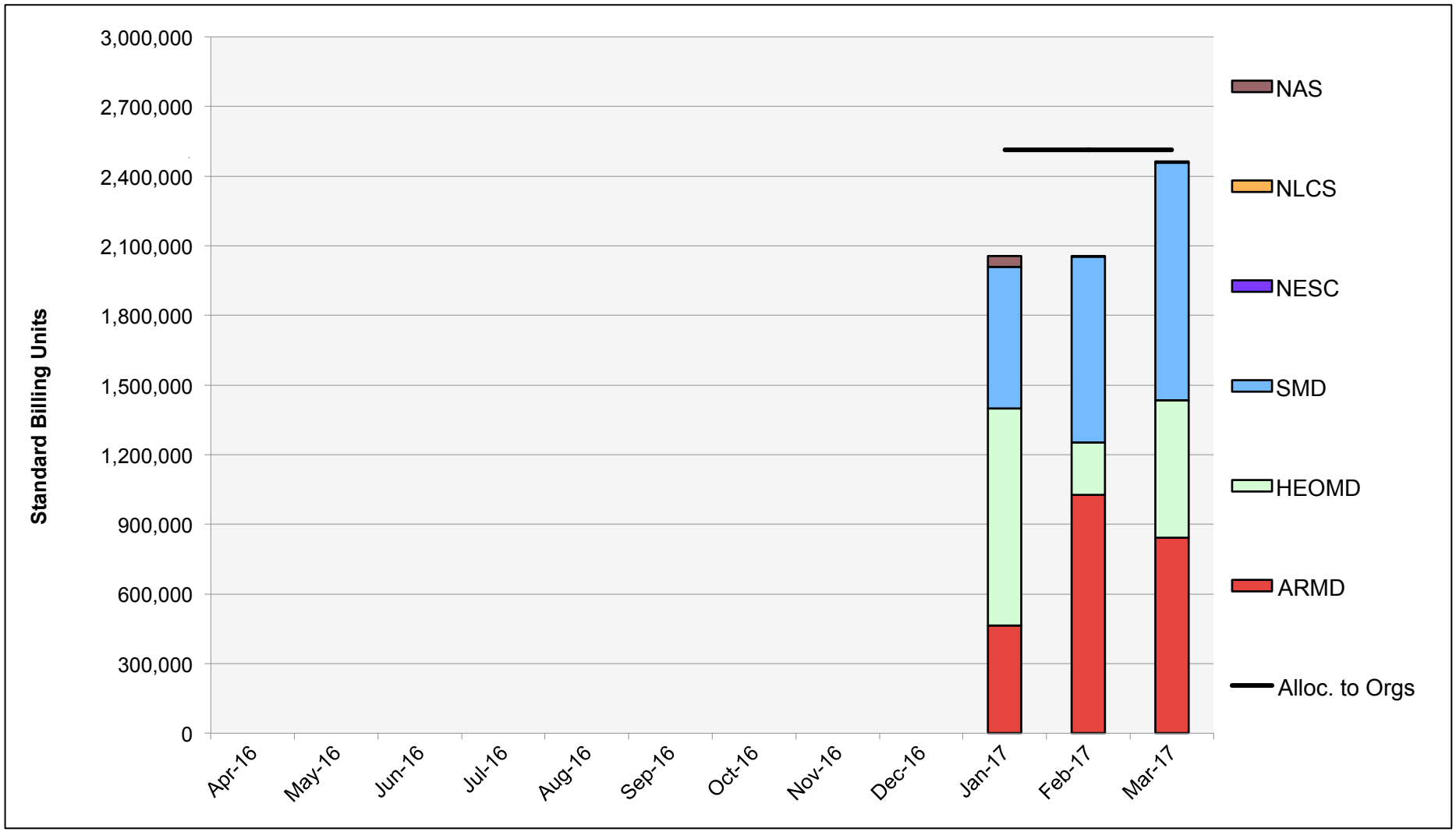
Pleiades:
Average Time to Clear All Jobs



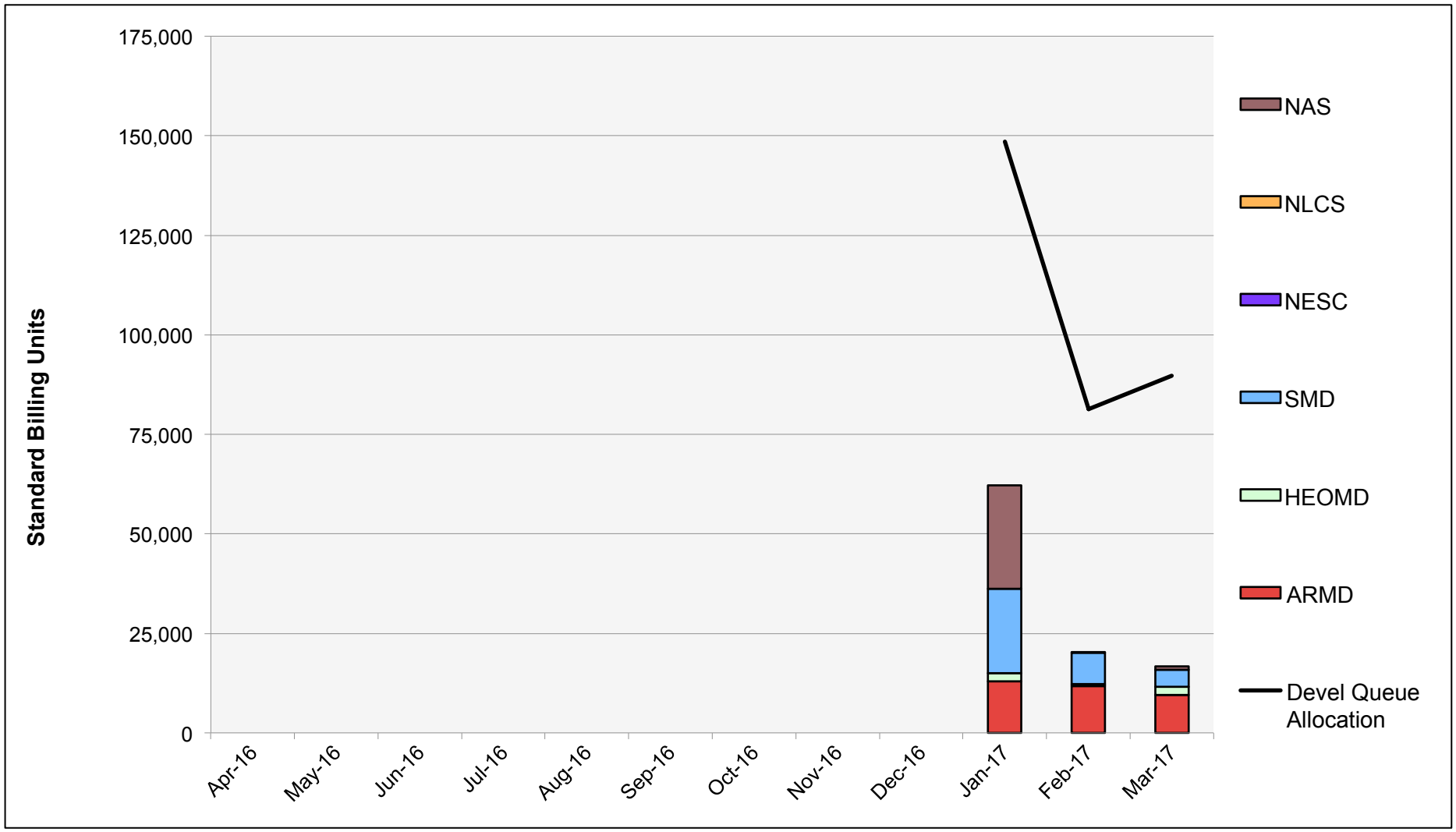
Pleiades:
Average Expansion Factor



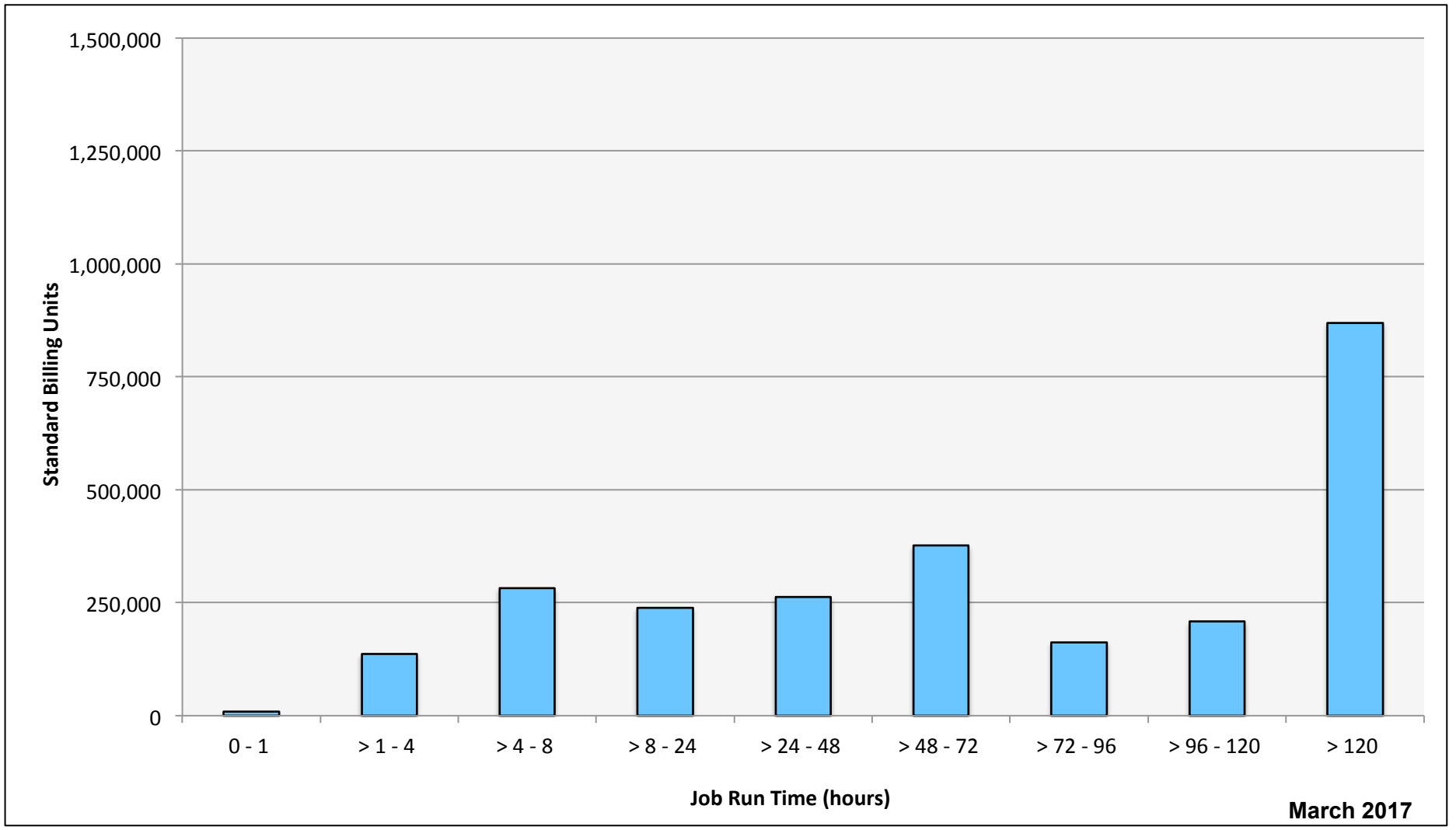
Electra:
SBUs Reported, Normalized to 30-Day Month



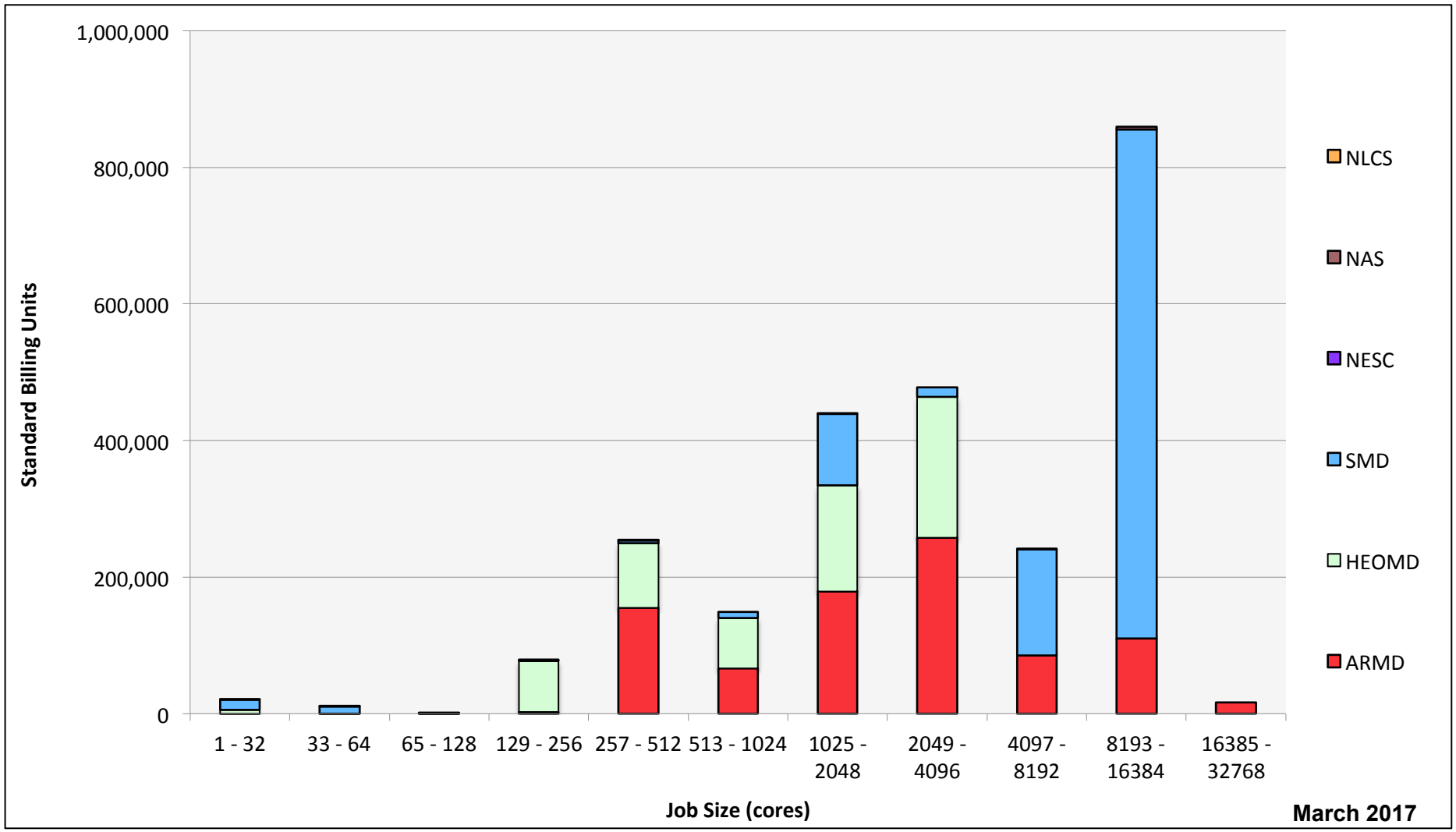
Electra:
Devel Queue Utilization



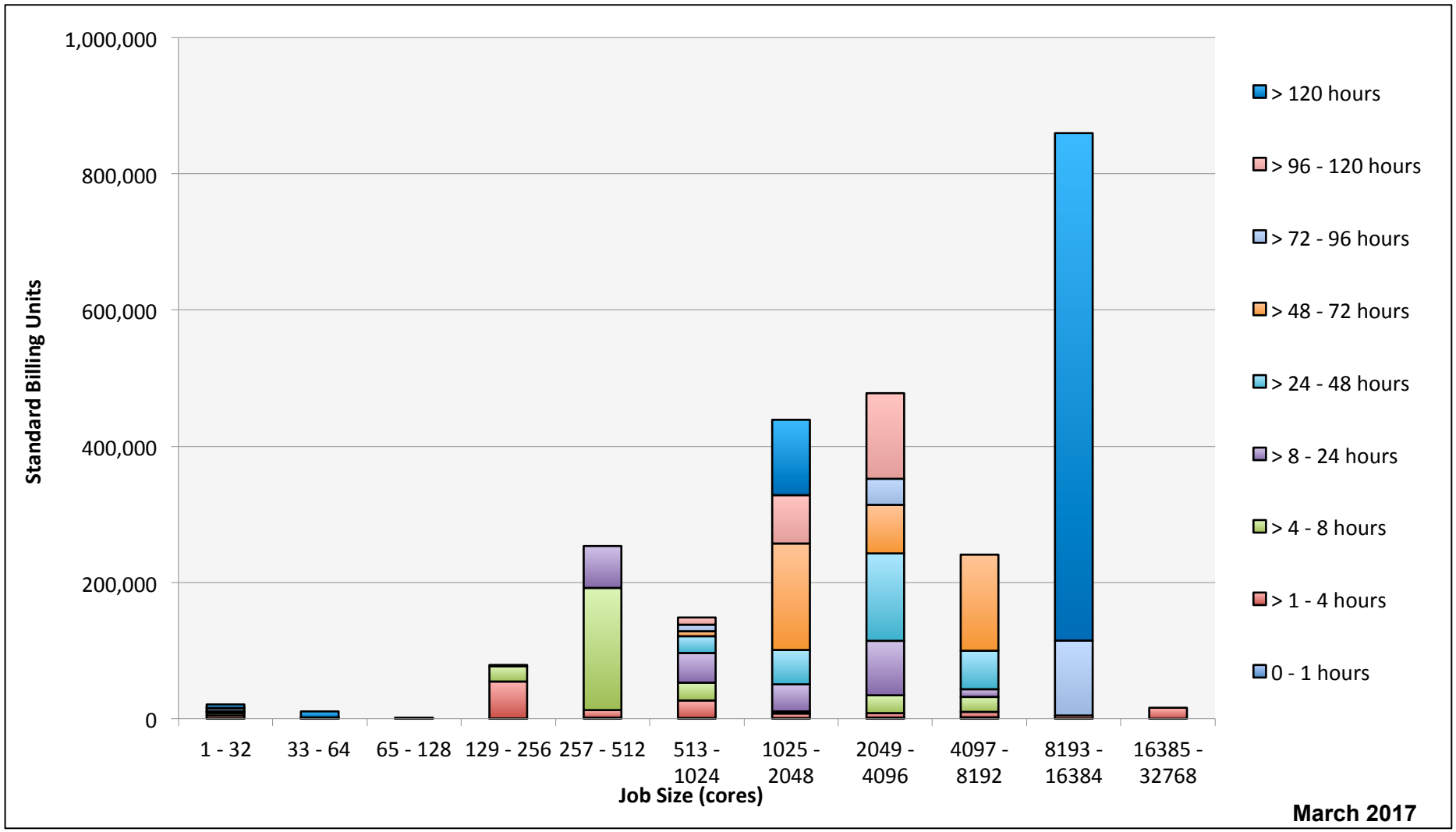
Electra:
Monthly Utilization by Job Length



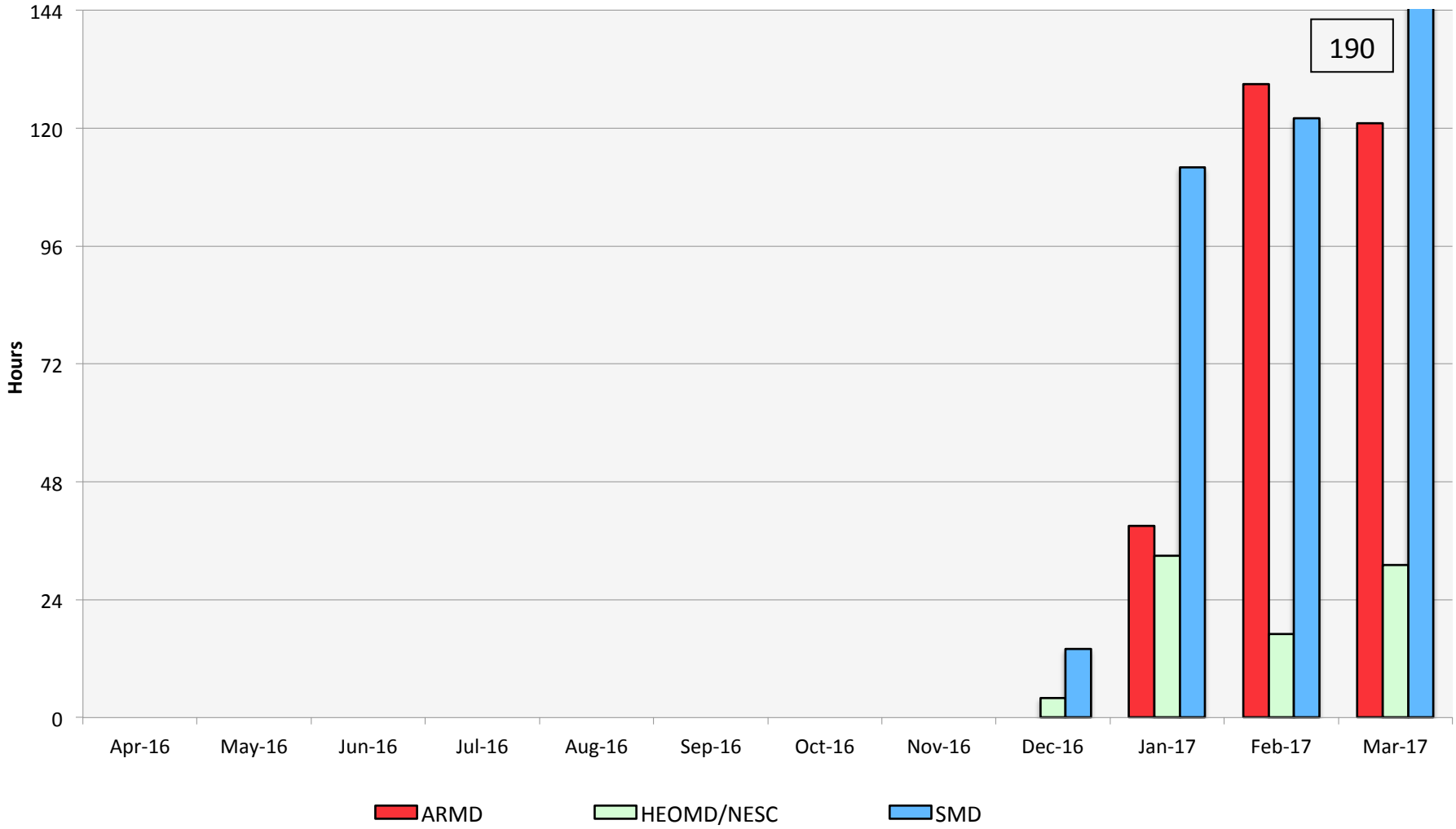
Electra:
Monthly Utilization by Size and Mission



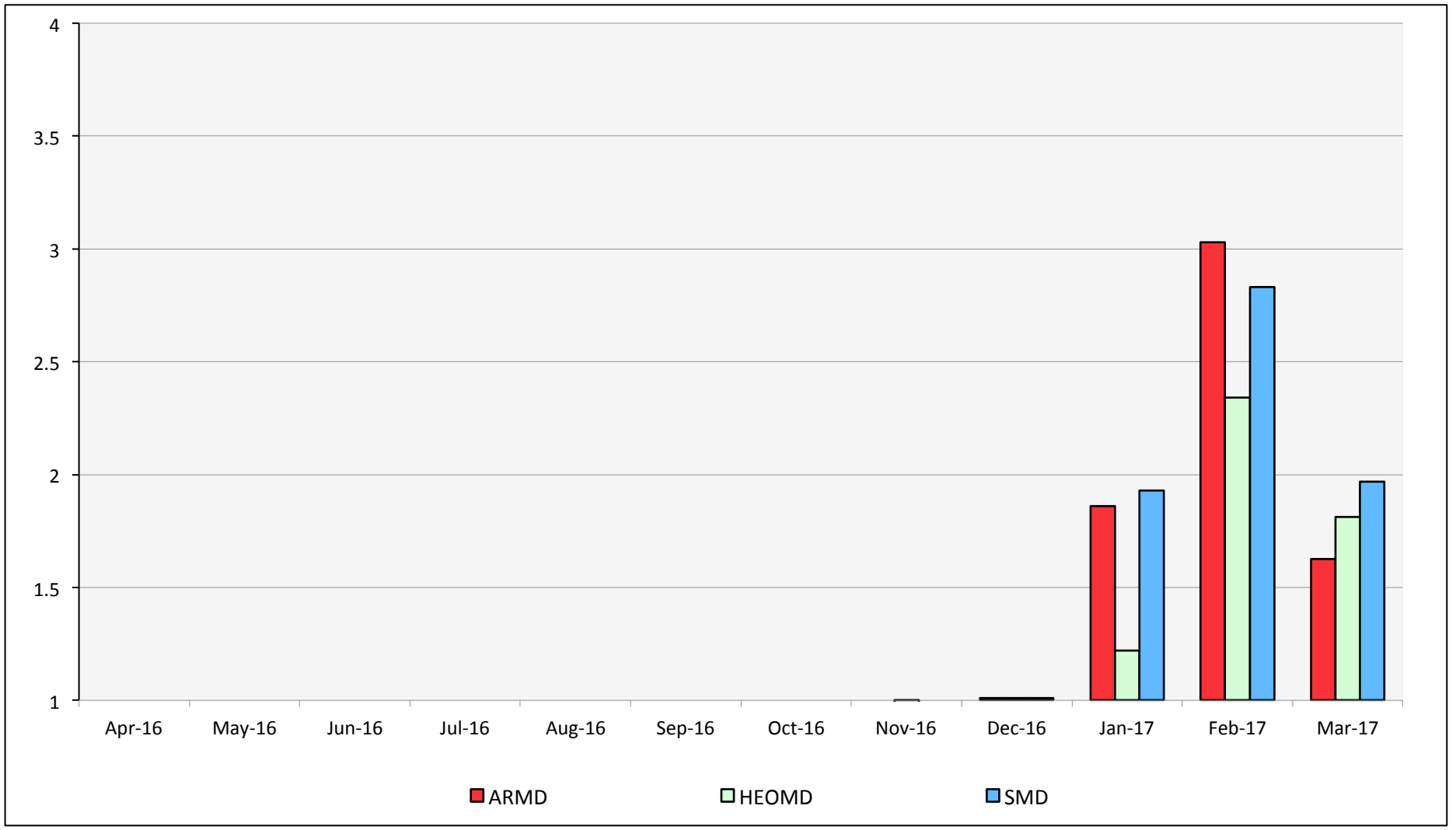
Electra:
Monthly Utilization by Size and Length



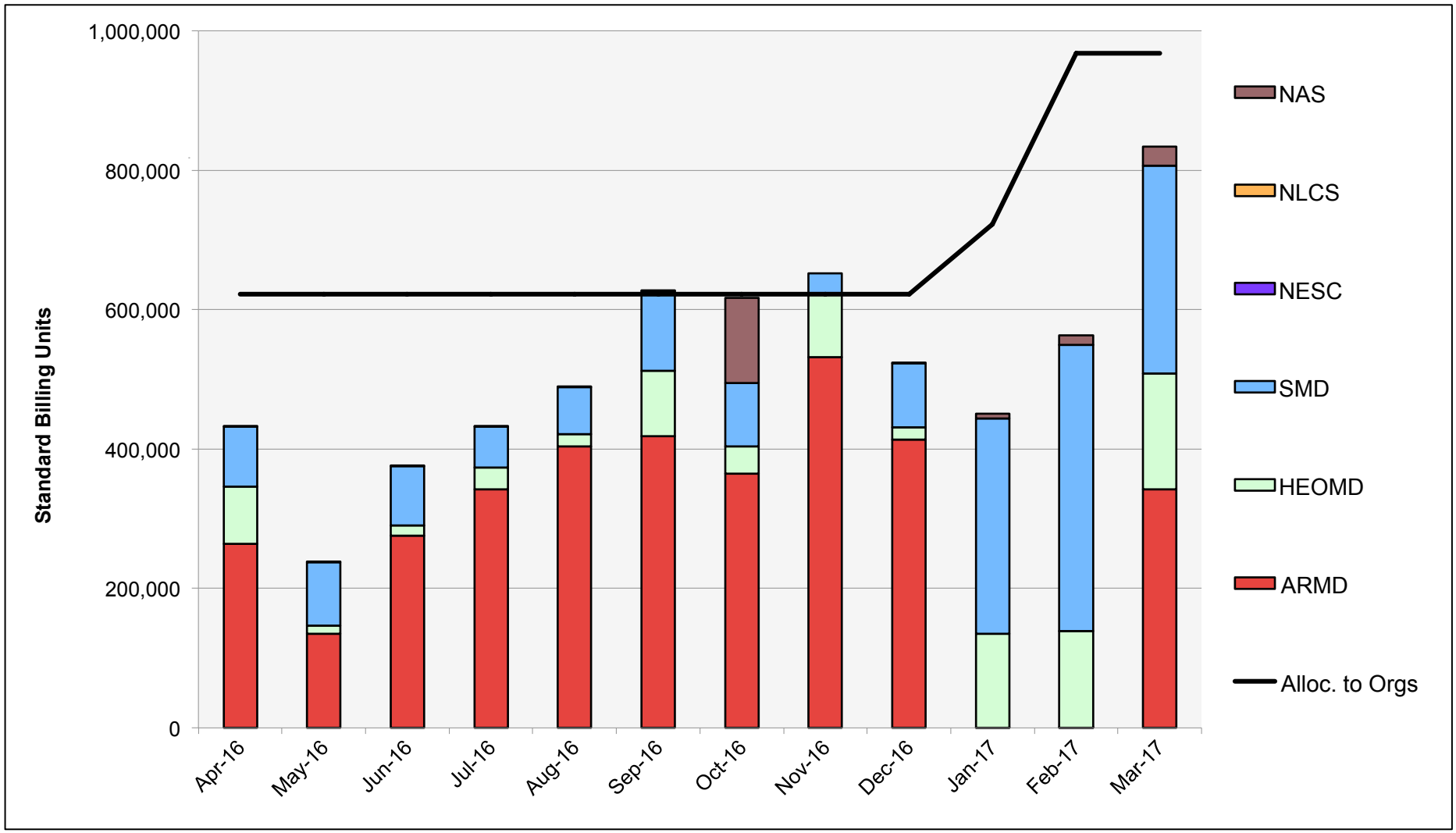
Electra:
Average Time to Clear All Jobs



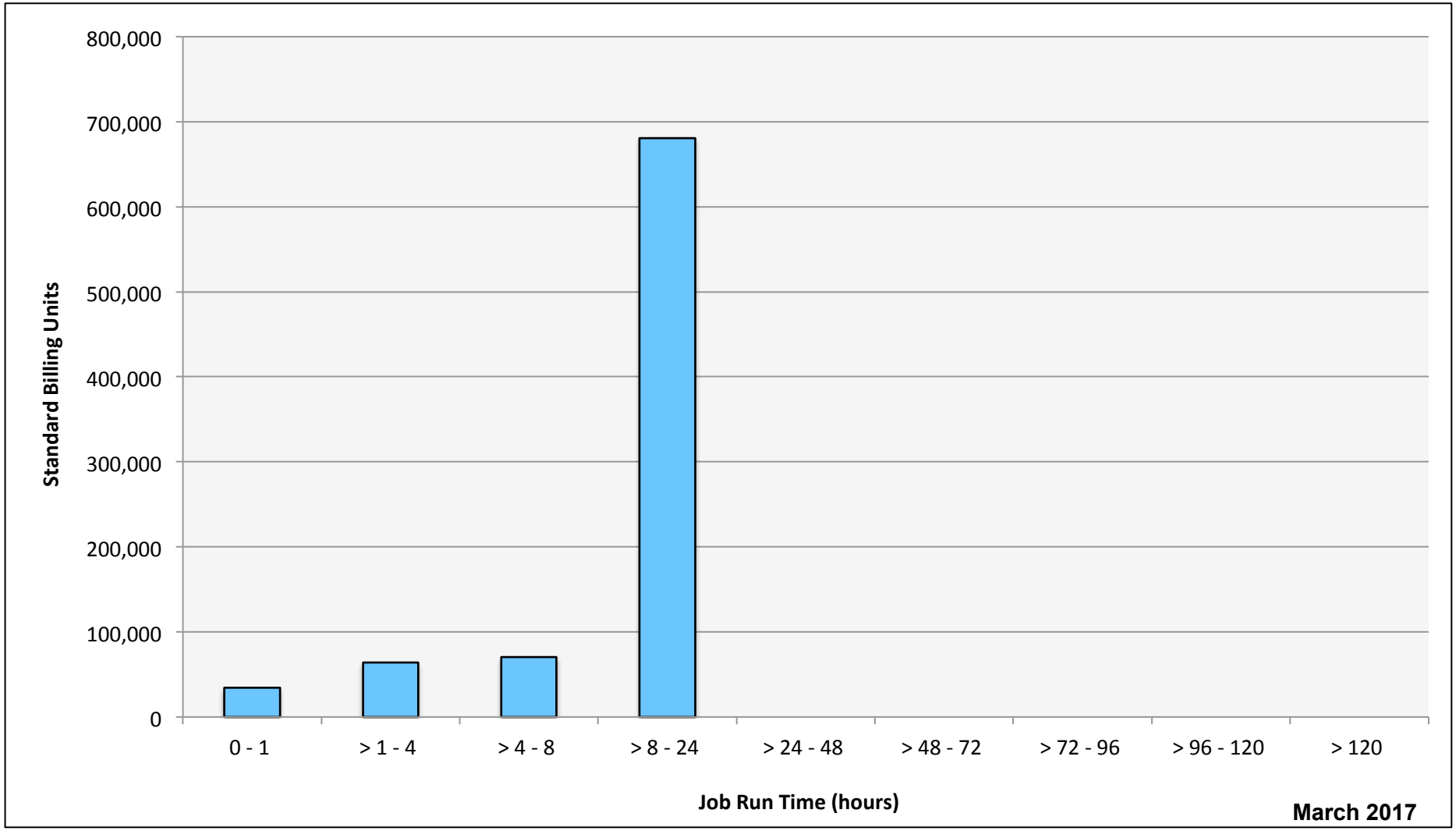
Electra:
Average Expansion Factor



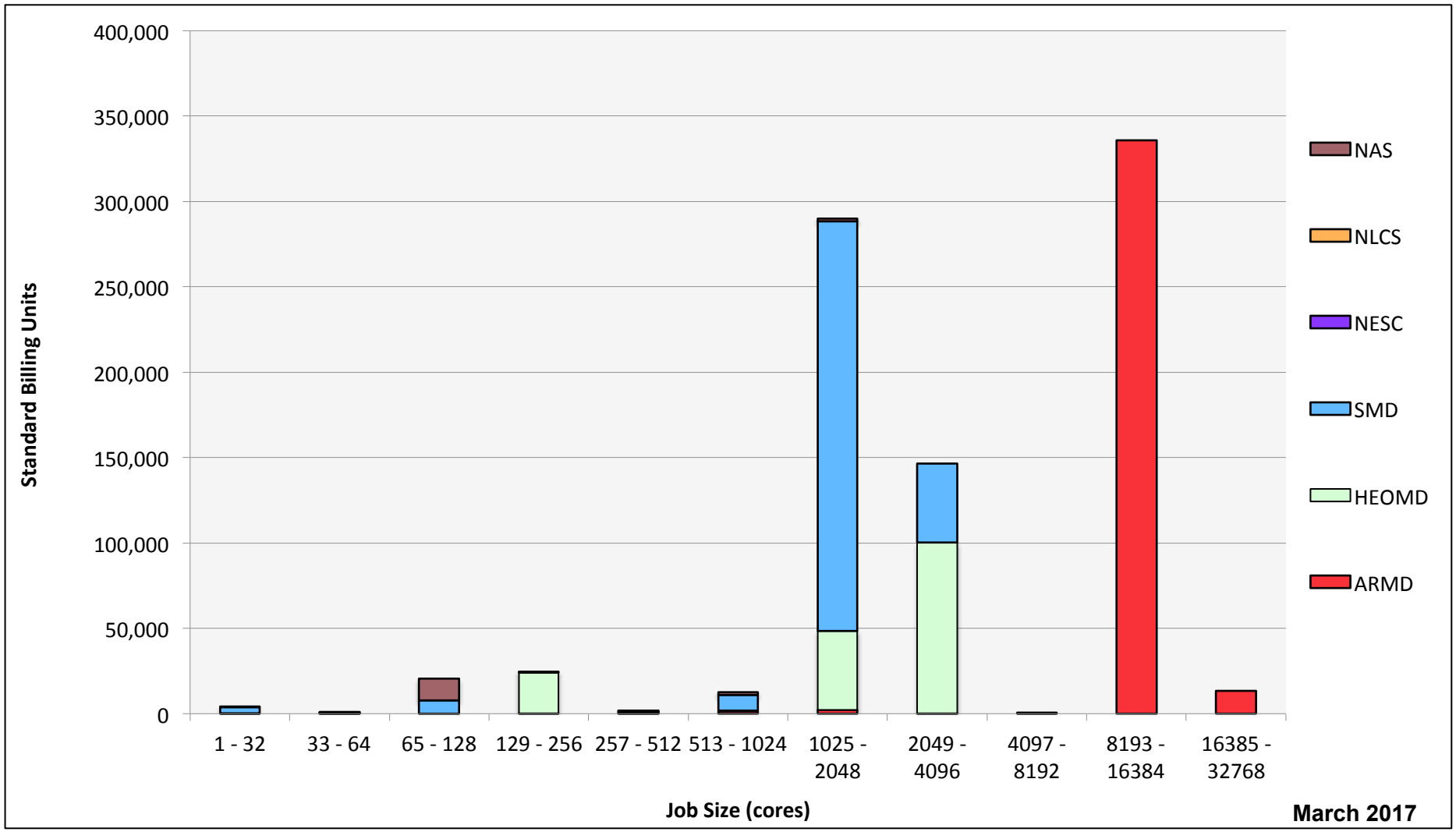
Merope:
SBUs Reported, Normalized to 30-Day Month



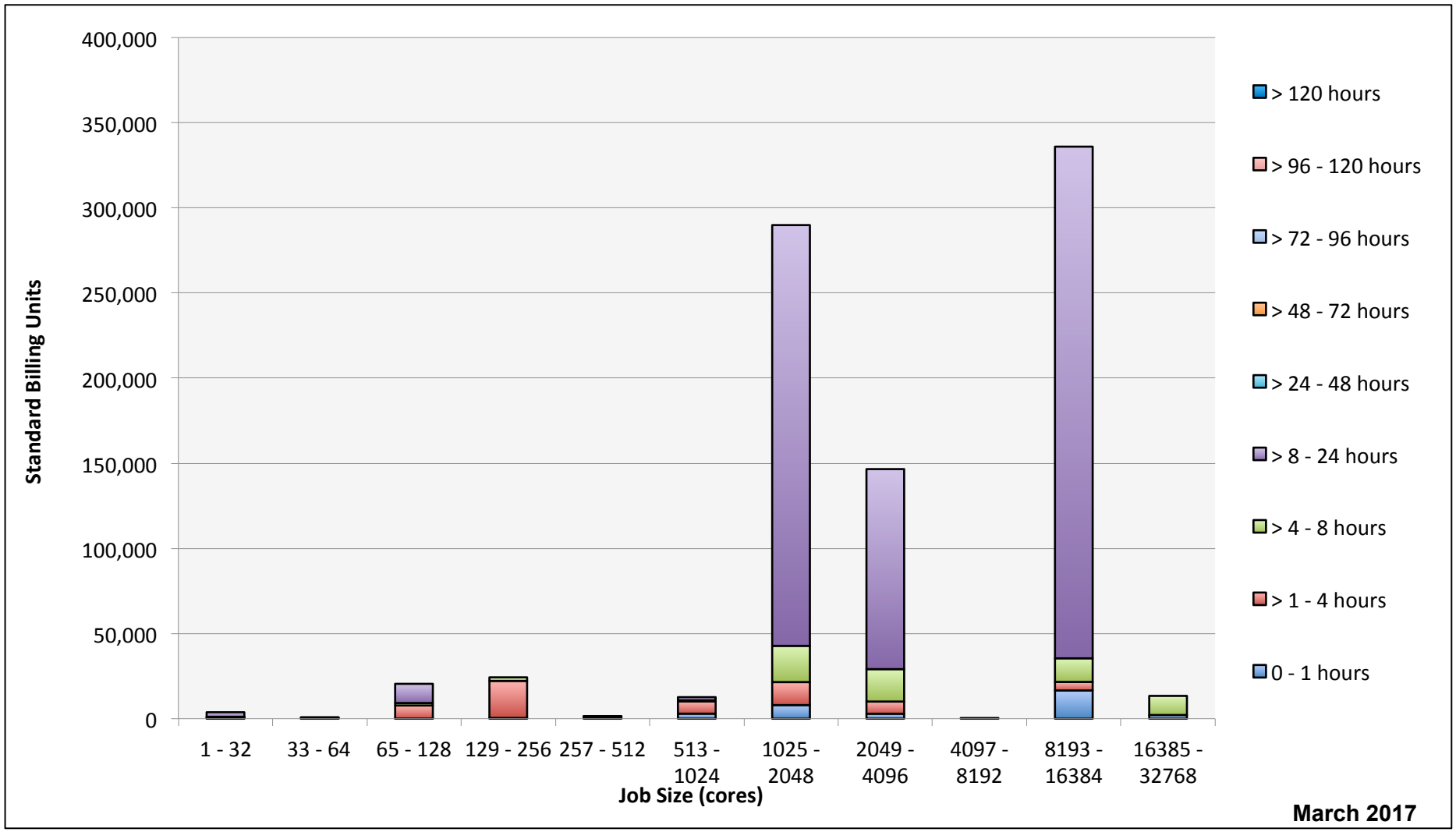
Merope:
Monthly Utilization by Job Length



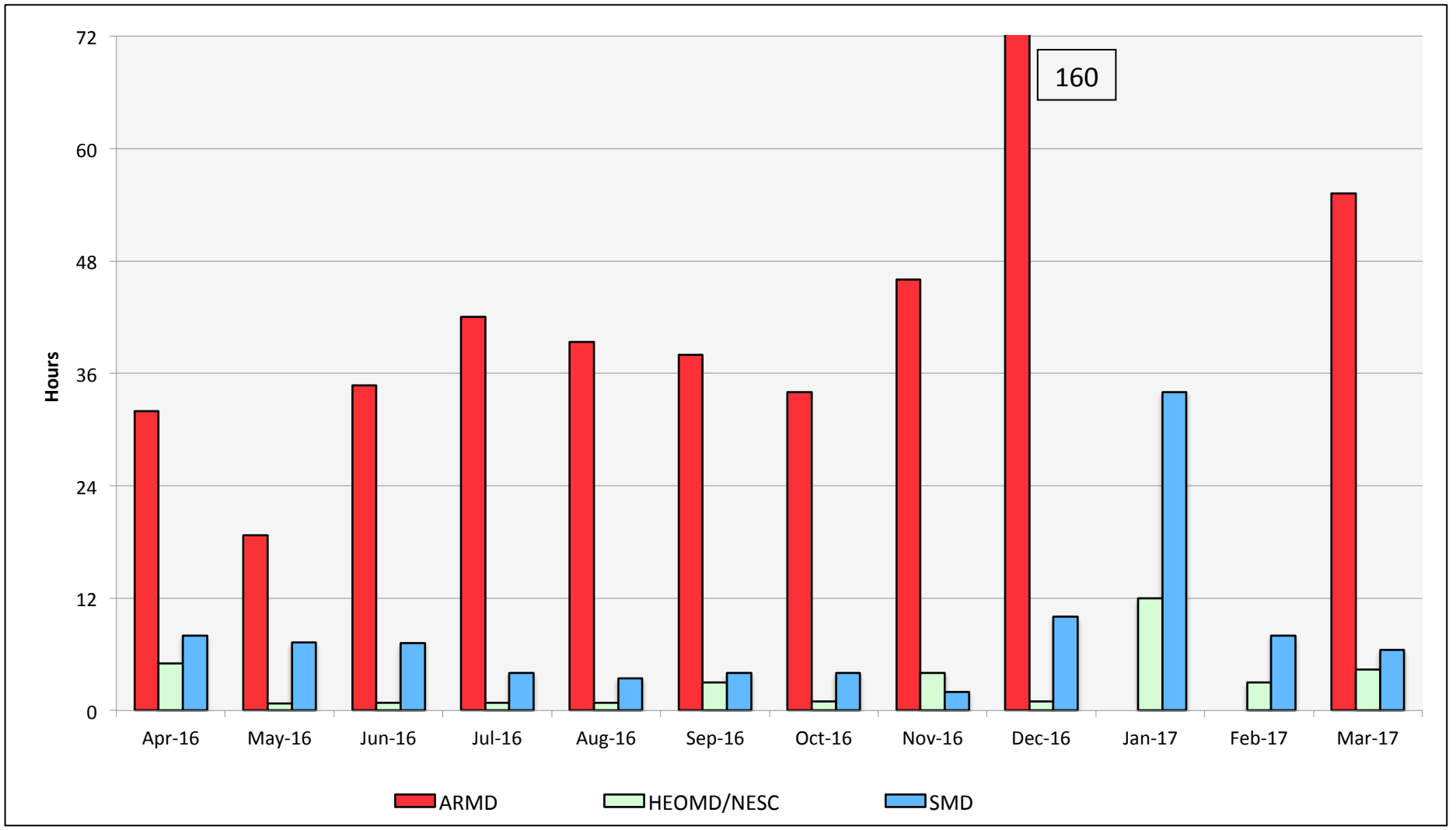
Merope:
Monthly Utilization by Size and Mission



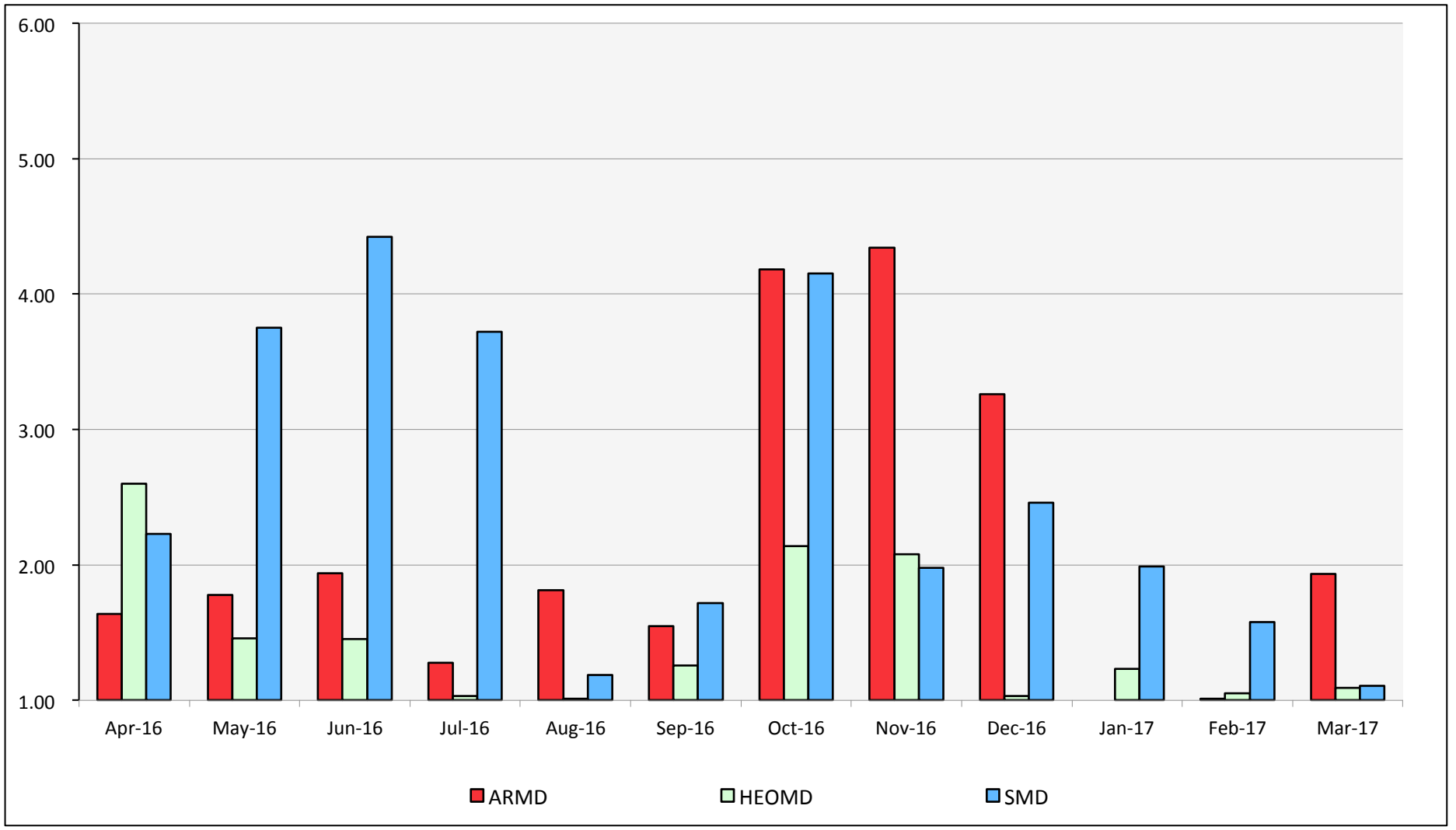
Merope:
Monthly Utilization by Size and Length



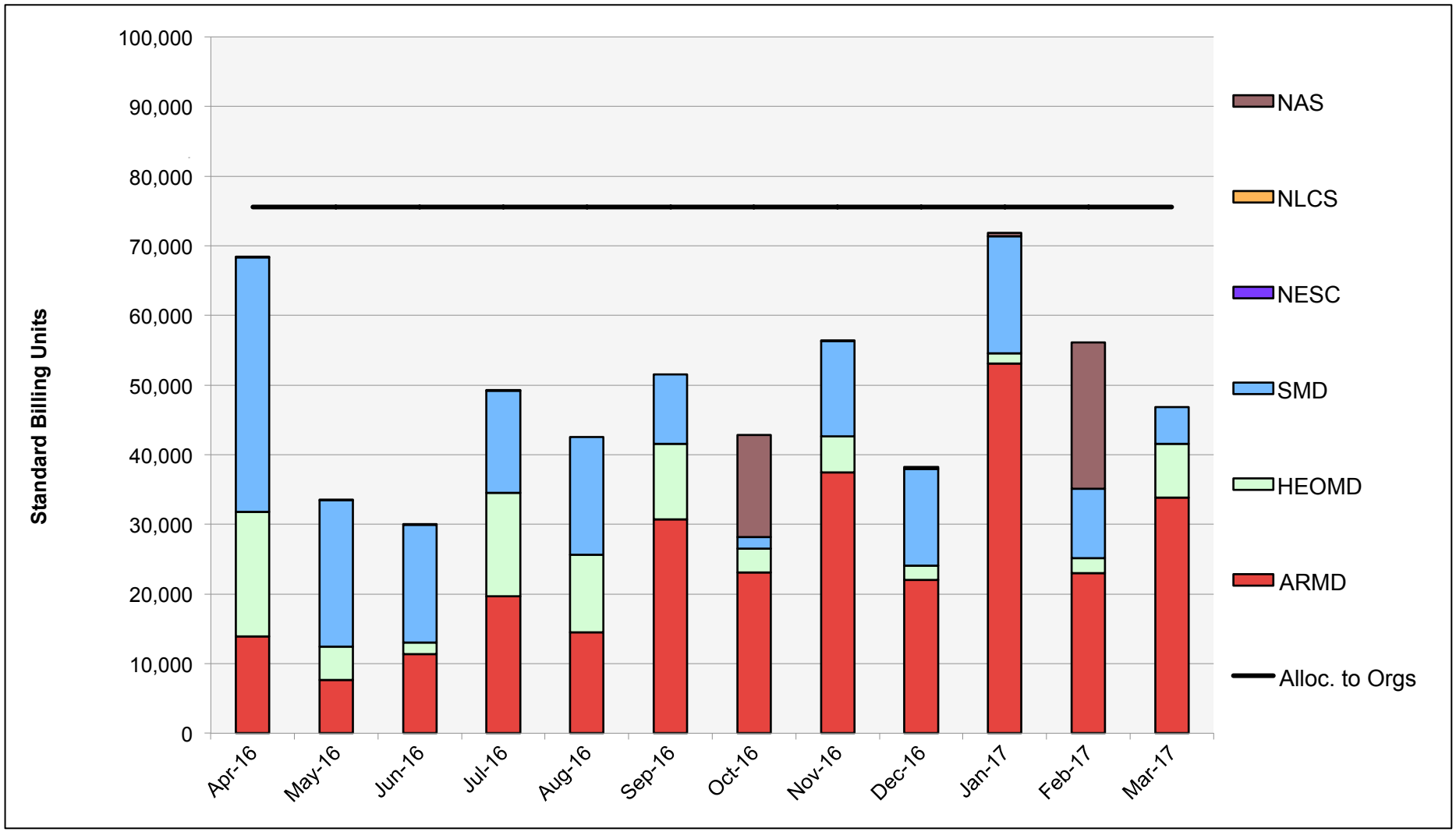
Merope:
Average Time to Clear All Jobs



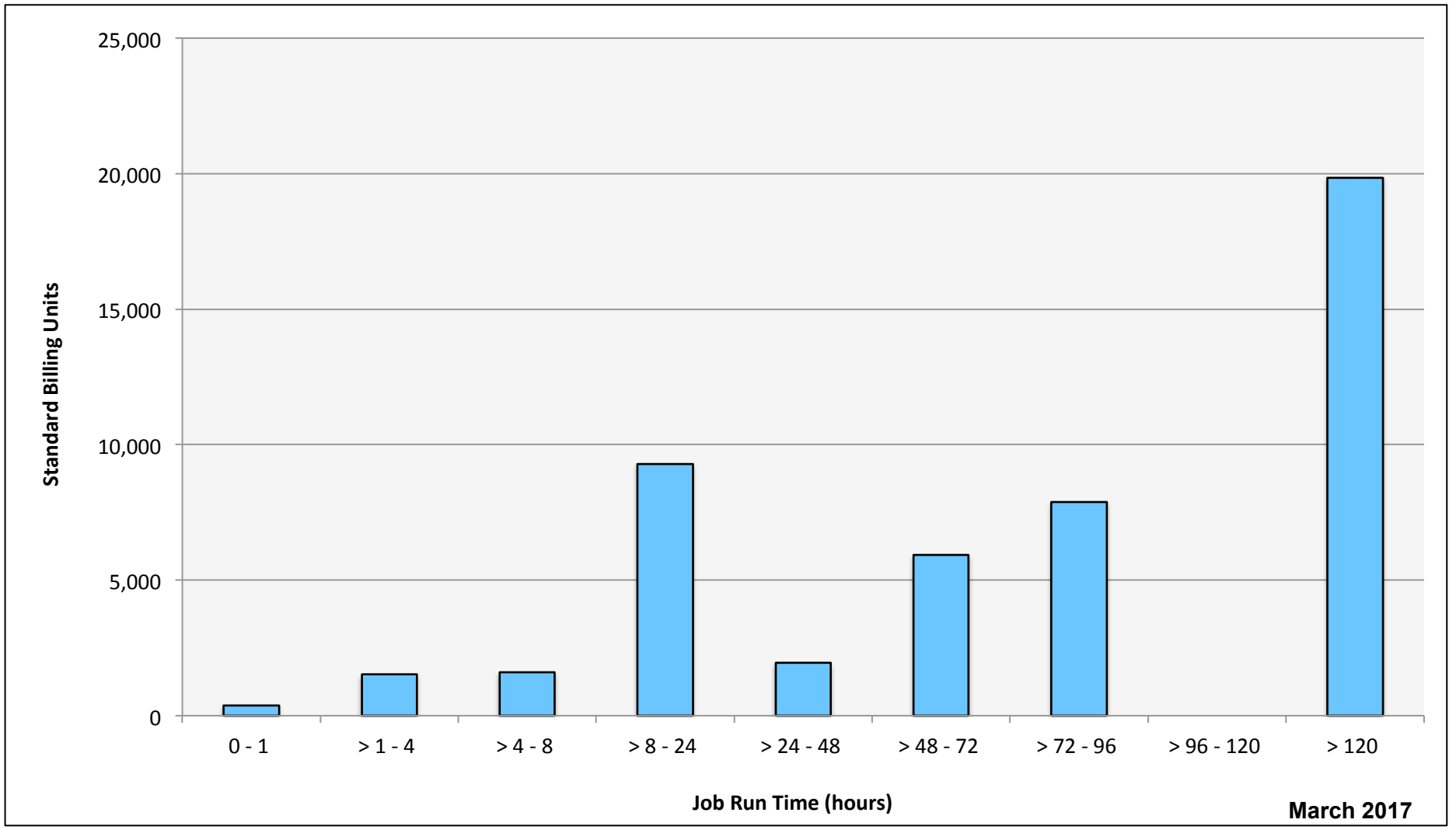
Merope:
Average Expansion Factor



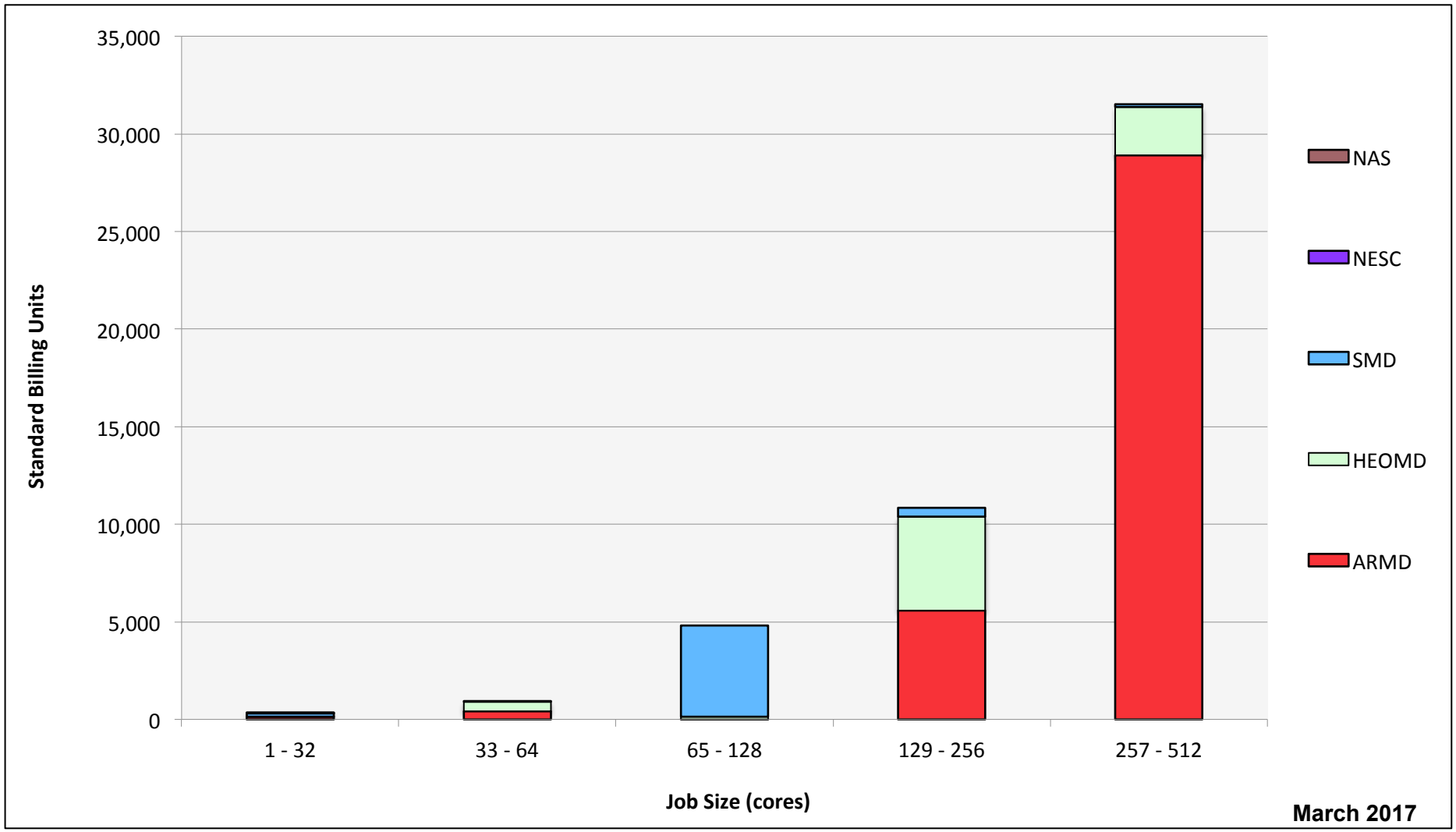
Endeavour:
SBUs Reported, Normalized to 30-Day Month



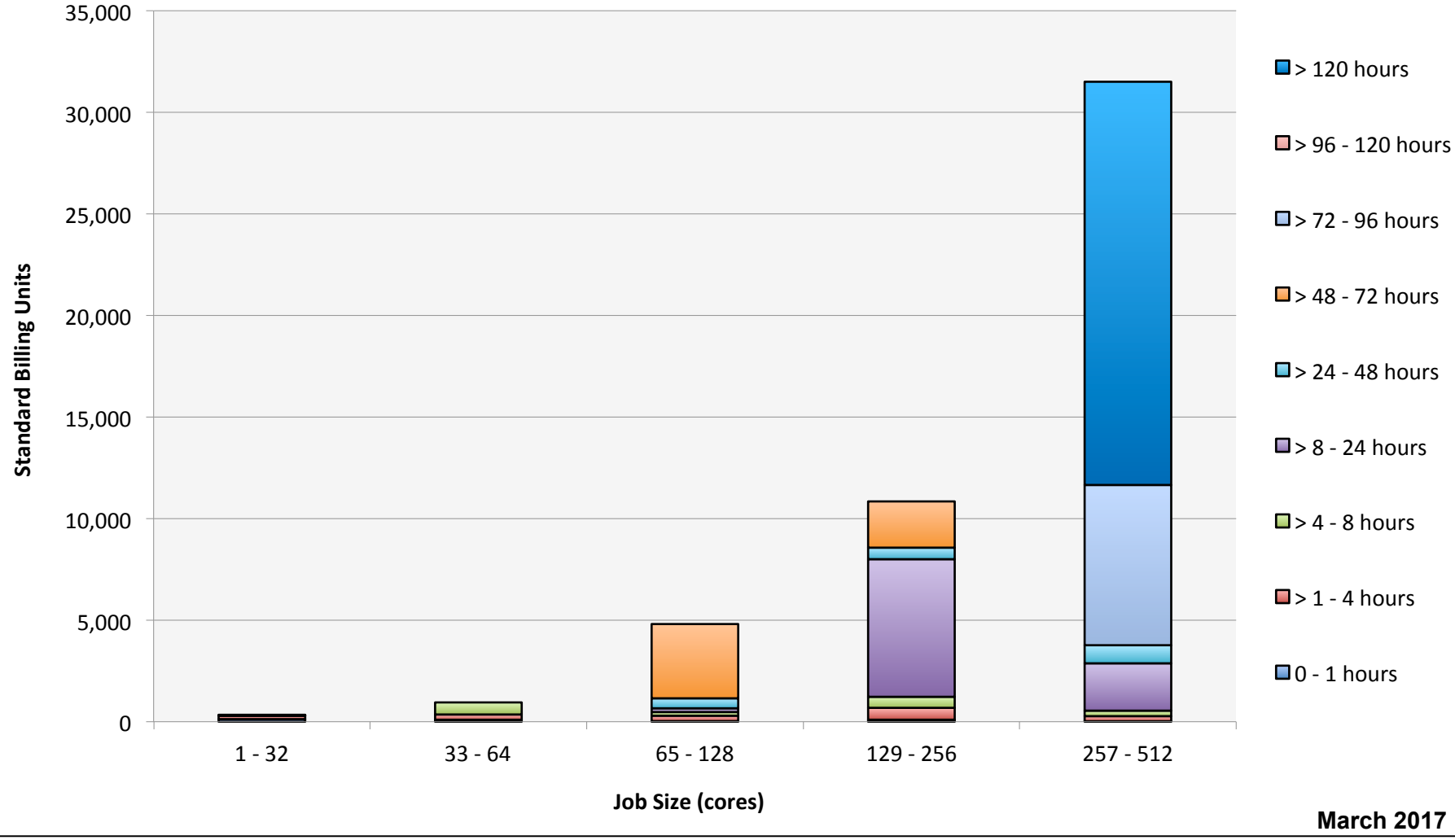
Endeavour:
Monthly Utilization by Job Length



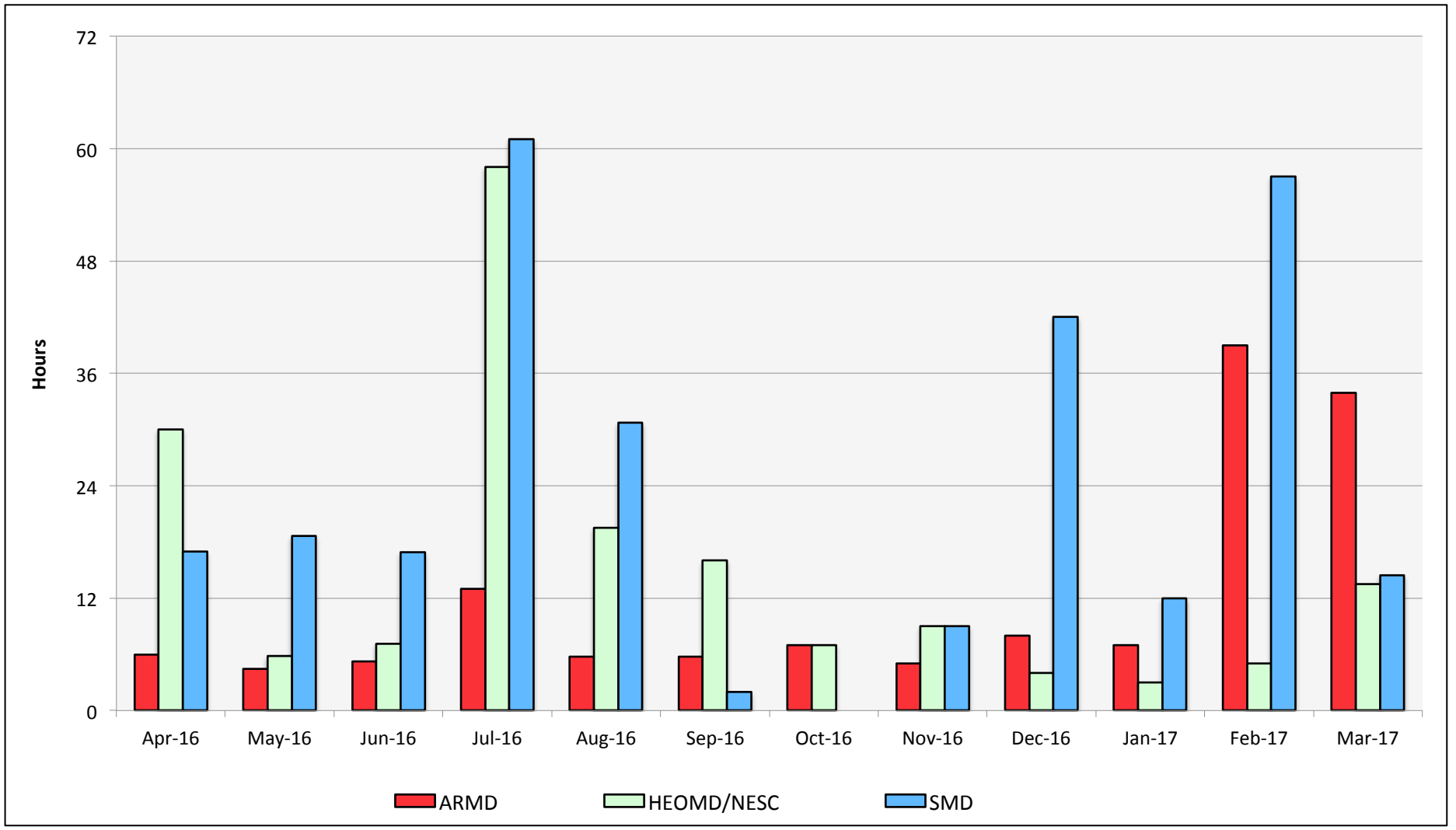
Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor